

Nuclear Polarized Hydrogen/Deuterium Molecules: Evidence, Production and for what they can be used

17.02.2015

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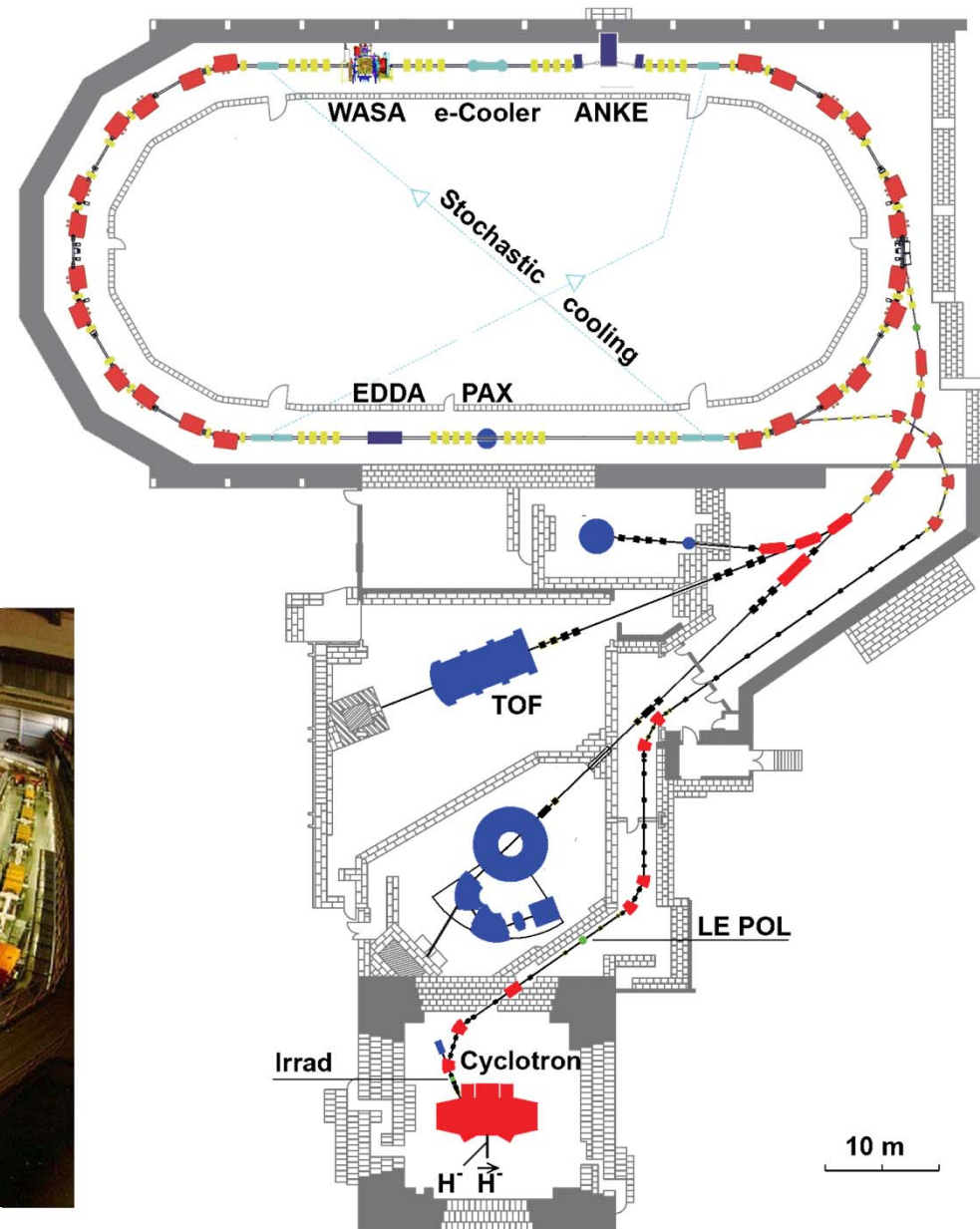
Outline

- **Polarized Internal Targets in Nuclear Physics**
- **The experimental Setup**
- **Important Details about H₂/D₂ Molecules**
- **Expected Results**
- **Experimental Results**
- **Conclusion and Outlook**

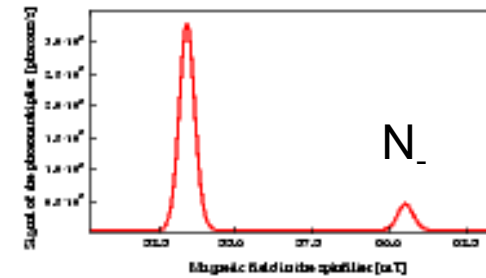
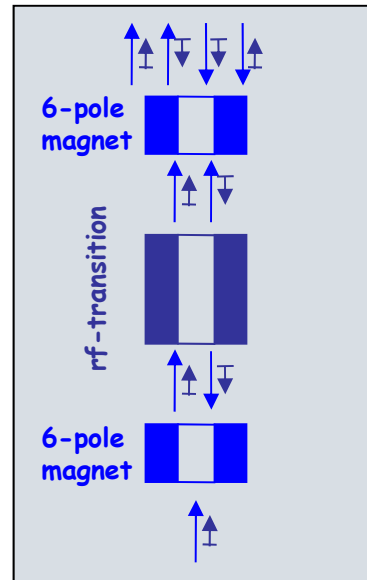
$$p, \vec{p}, d, \vec{d}$$

with momenta up to 3.7 GeV/c

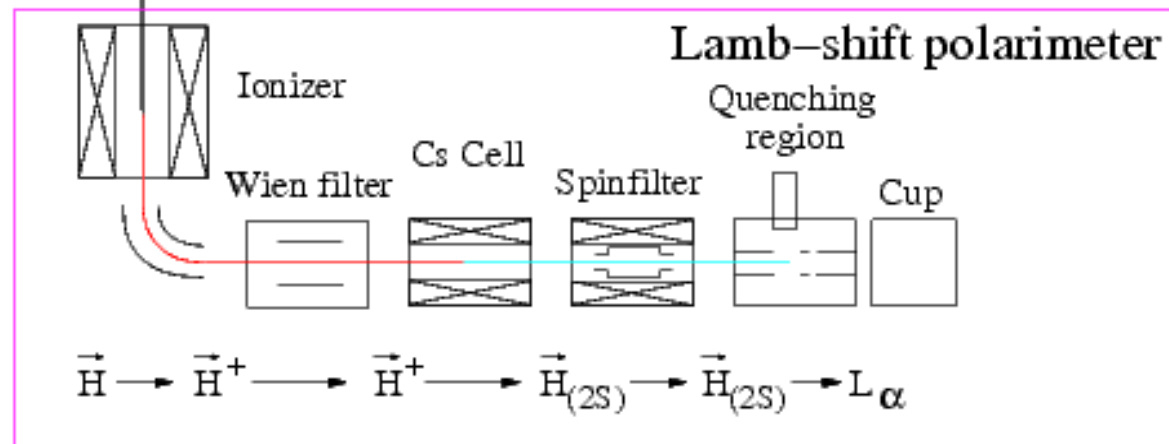
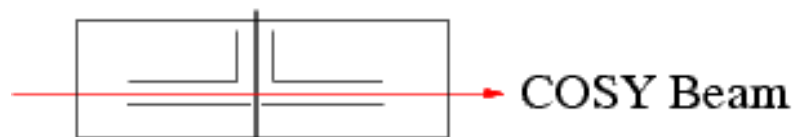
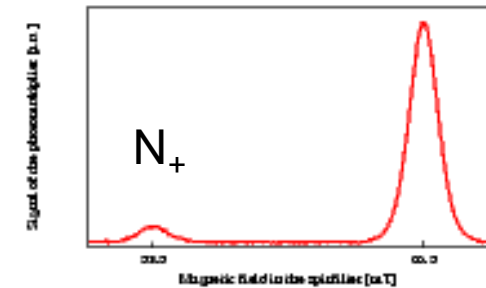
- **internal experiments** –
with the circulating beam
- **external experiments** –
with the extracted beam



ABS and Lamb-shift polarimeter



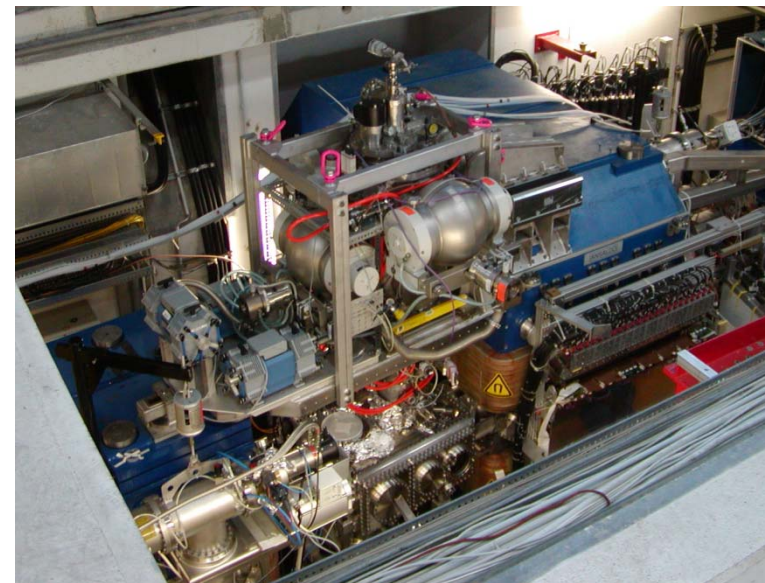
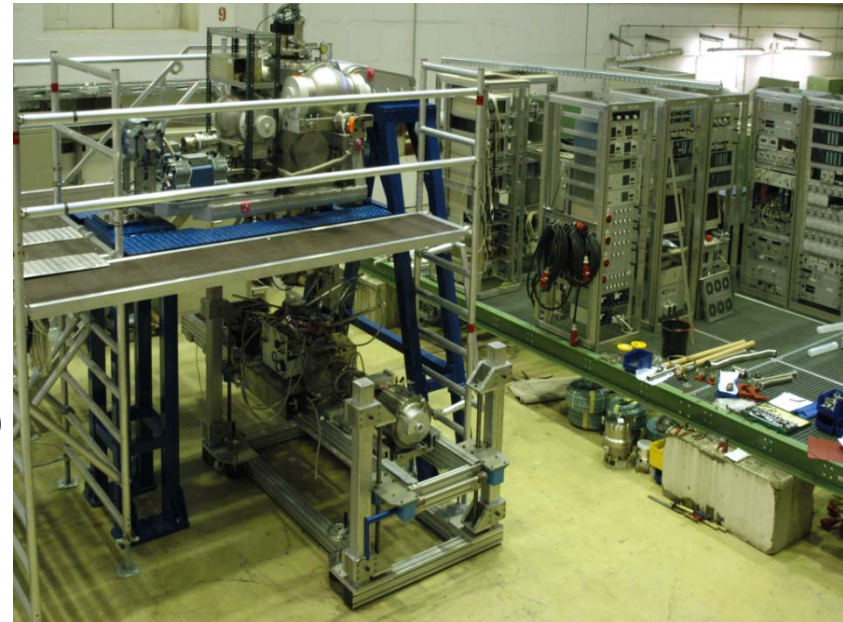
$$P = \frac{N_+ - N_-}{N_+ + N_-}$$



PIT @ ANKE/COSY

Main parts of a PIT:

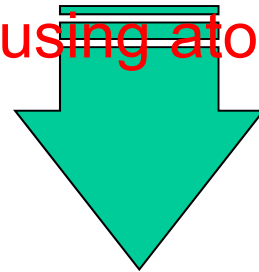
- **Atomic Beam Source**
 - Target gas
hydrogen or **deuterium**
 - H beam intensity (2 hyperfine states)
 $8.2 \cdot 10^{16}$ atoms / s
 - Beam size at the interaction point
 $\sigma = 2.85 \pm 0.42$ mm
 - Polarization for hydrogen atoms
 $P_Z = 0.89 \pm 0.01$ (HFS 1)
 $P_Z = -0.96 \pm 0.01$ (HFS 3)
- **Lamb-Shift Polarimeter**
- **Storage Cell**



Polarized H₂ Molecules

- Beam intensities of conventional ABS barely reach $\sim 10^{17}$ at/s
⇒ target density $d_t \sim 10^{14}$ at/cm² (typical T-shaped storage cell)
- Depolarization at low T of storage cell don't allow further cooling

Performance of PIT using atomic beams saturates!



New storage cell materials

Polarized molecules?

Polarized H₂ Molecules

Measurements from NIKHEF, IUCF, HERMES show that recombined molecules retain fraction of initial nuclear polarization of atoms!

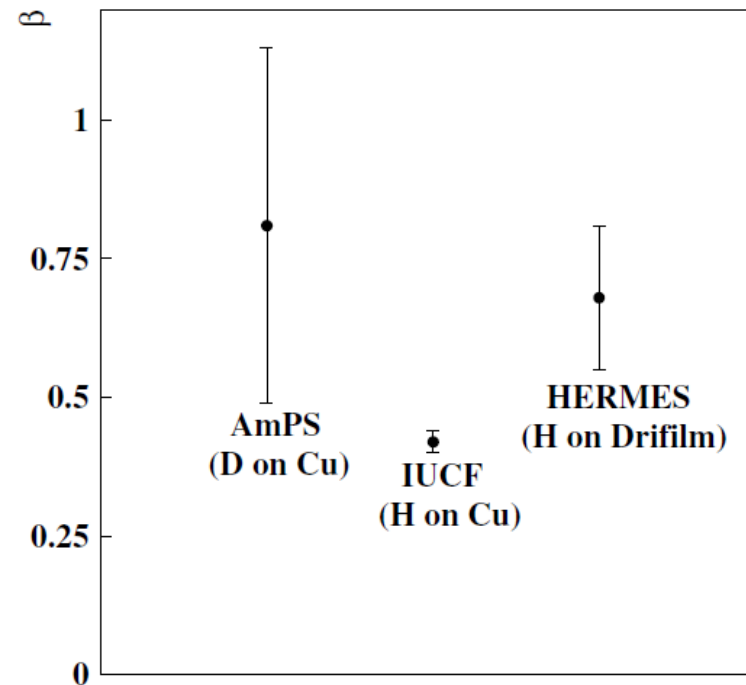


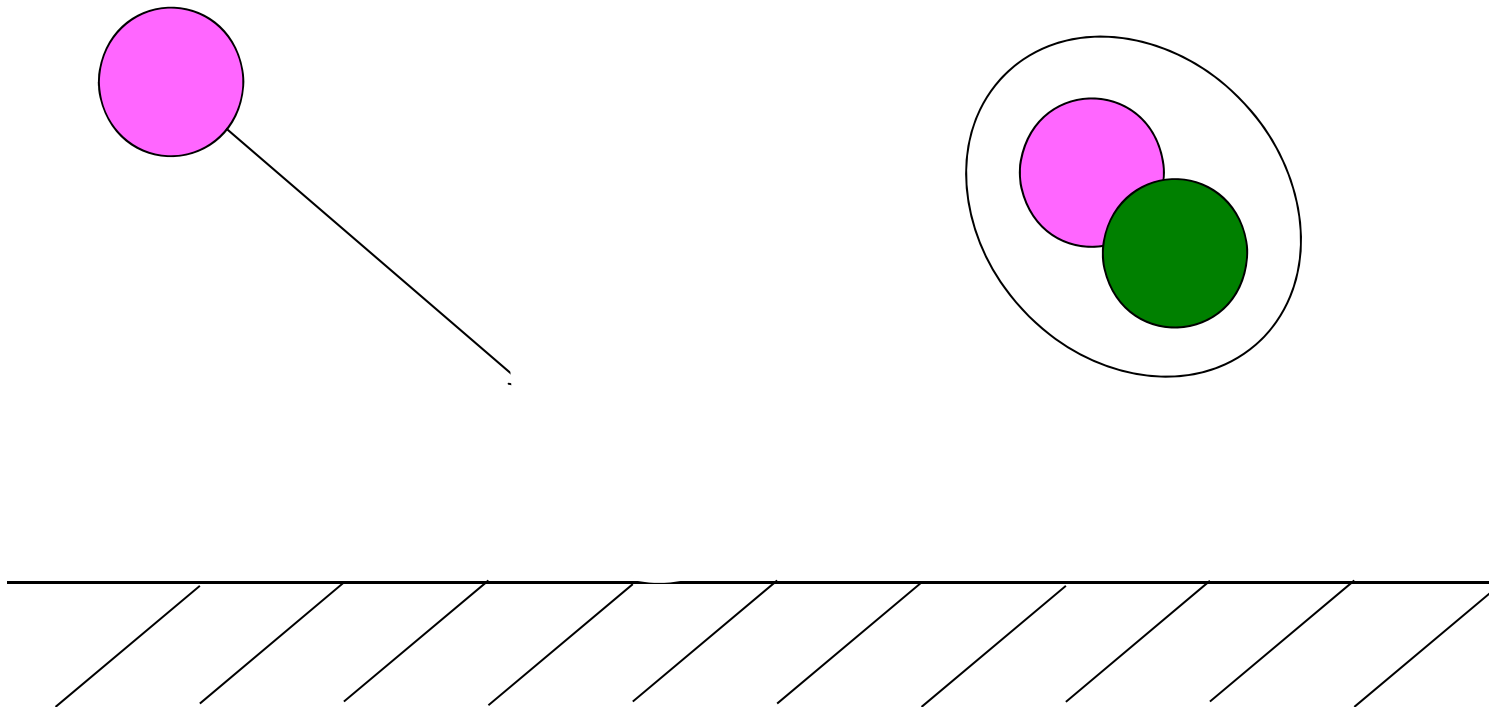
Fig. 2. Summary of the existing measurements of the nuclear polarization of recombined molecules. The newly obtained HERMES measurement at 260 K with a holding field of 330 mT is compared to the measurement by AmPS and IUCF obtained at room temperature and magnetic holding fields of 28 mT and 440 mT respectively.

The HERMES Collaboration; Eur. Phys. J. D **29**, 21–26 (2004)
DOI: 10.1140/epjd/e2004-00023-5

Polarized H₂ Molecules

Eley-Rideal Mechanism

$$P_m = 0.5$$

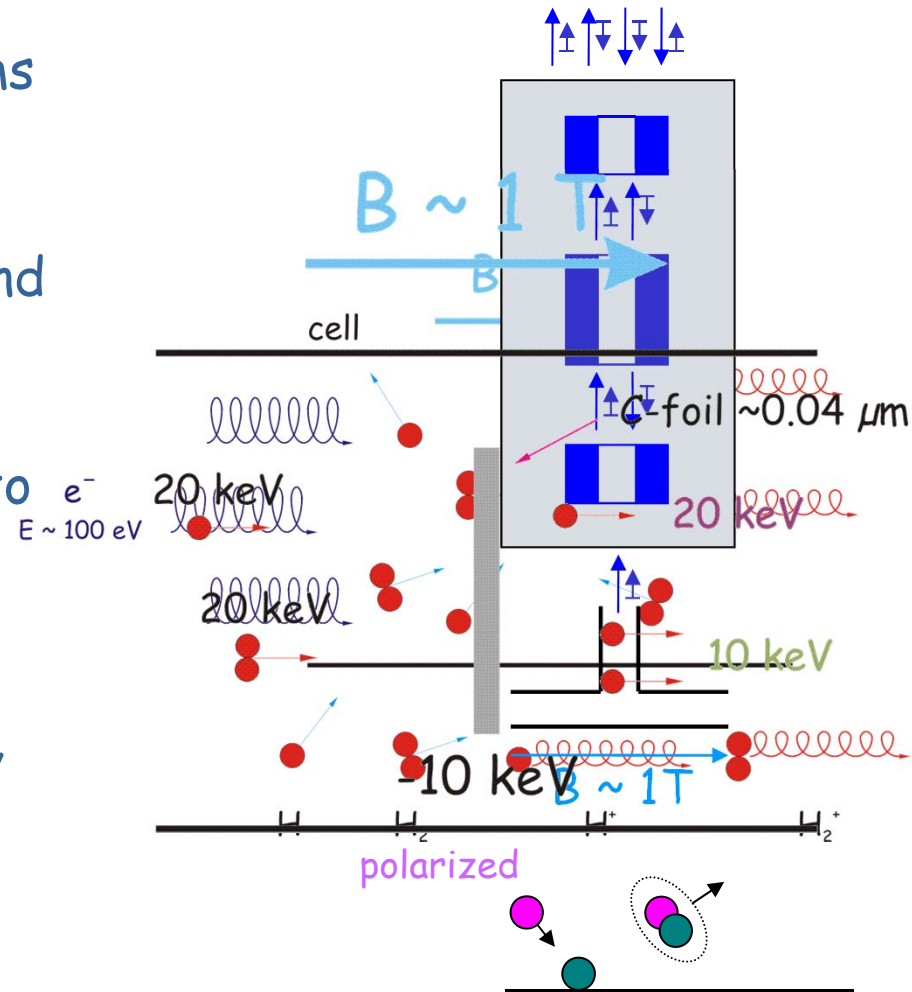


Is there a way to increase P_m

(surface material, T, B etc)?

The original idea

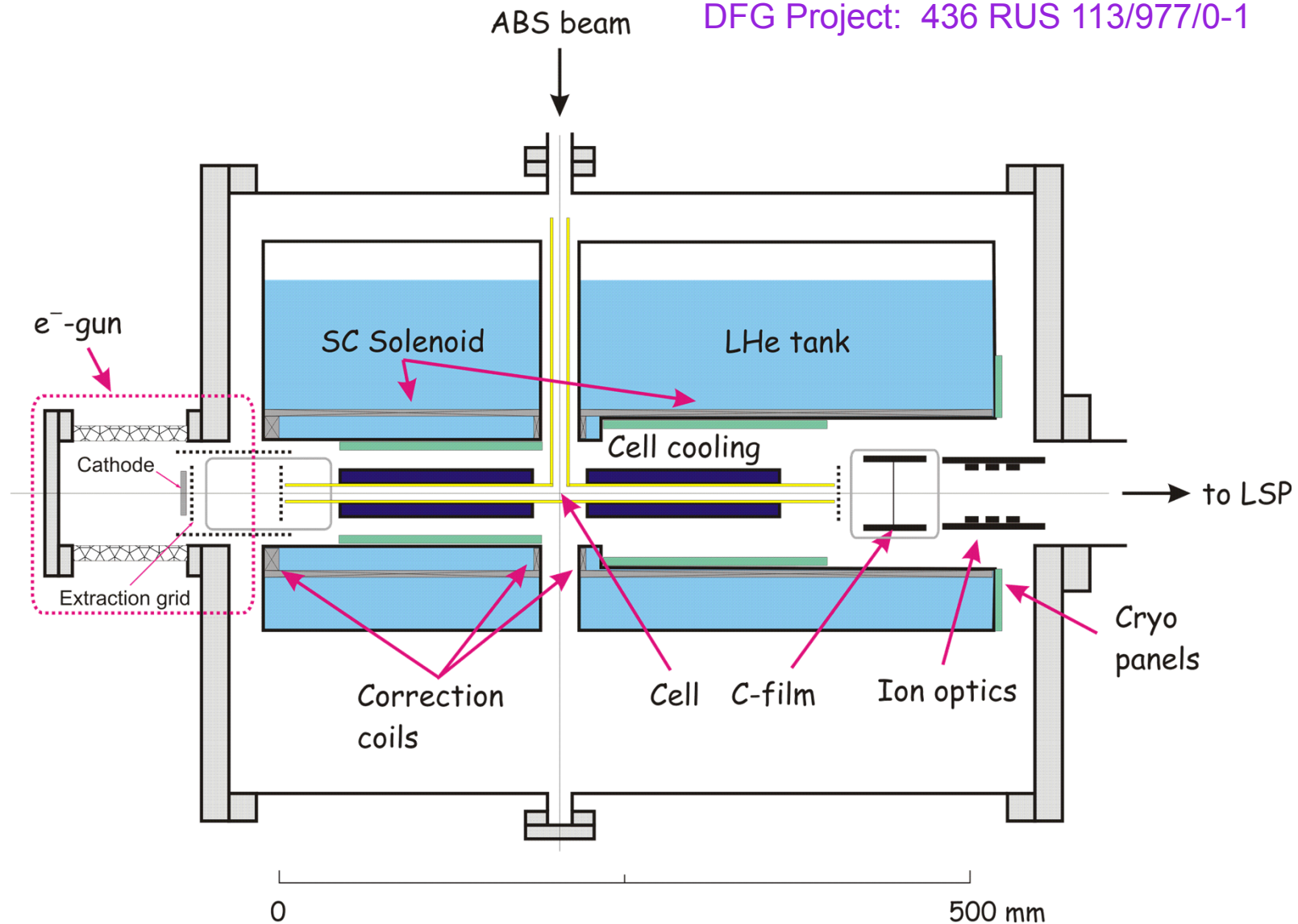
- Recombination of polarized atoms into molecules
- Conversion of polarized atoms and molecules into ions
- Conversion of H_2^+ and H^+ ions into protons with different energy (suggested by W.Haeberli)
- Separation of protons by energy
- Measurement of proton polarization in LSP



The experimental Setup

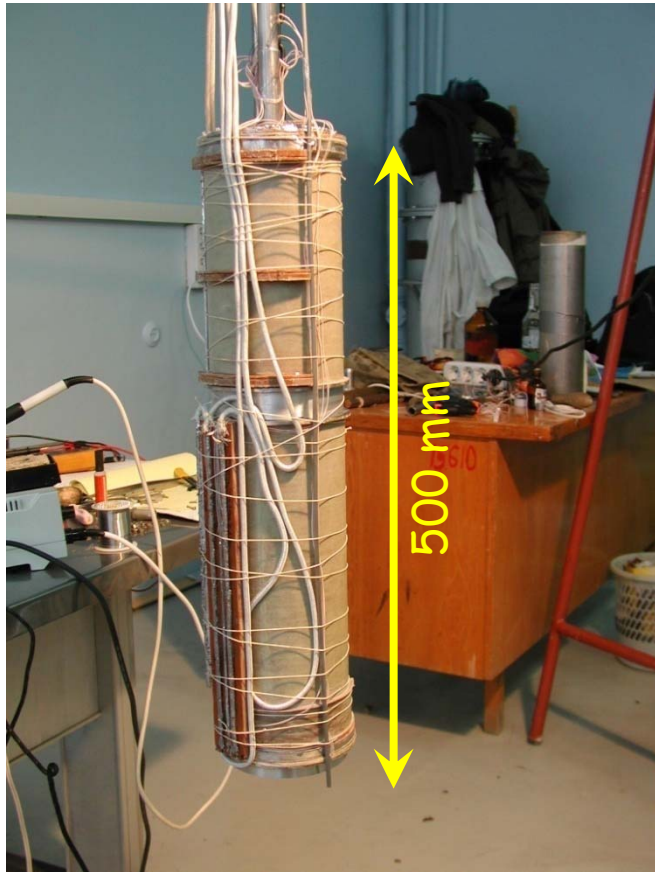
ISTC Project # 1861 PNPI, FZJ, Uni. Cologne

DFG Project: 436 RUS 113/977/0-1

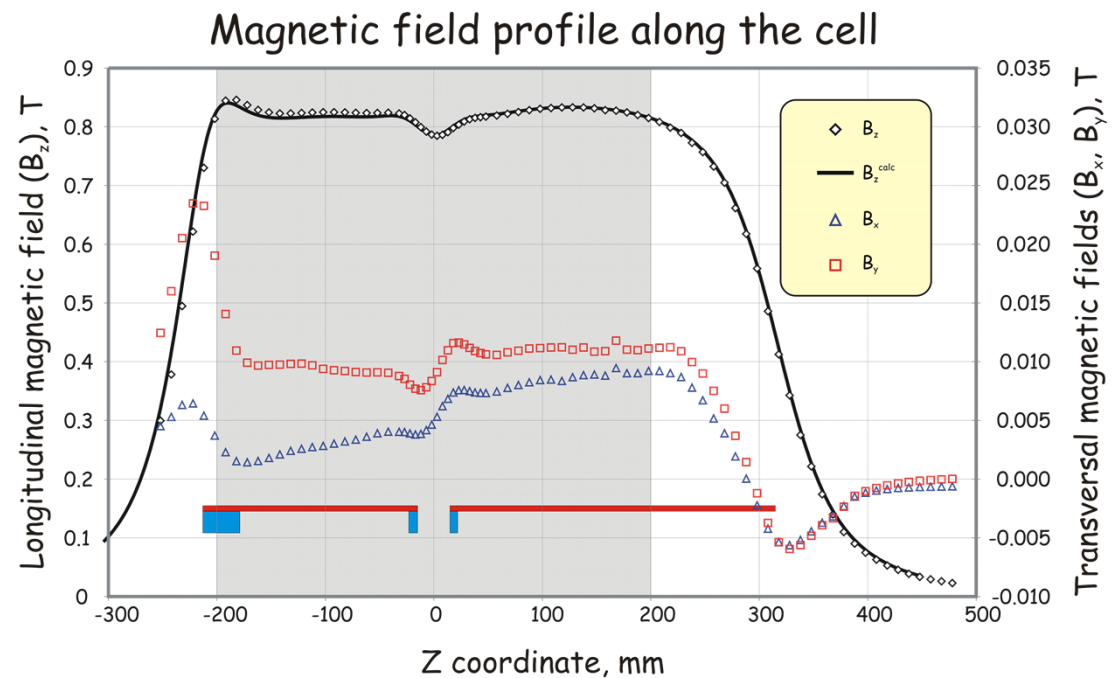


The experimental Setup

Superconducting Solenoid

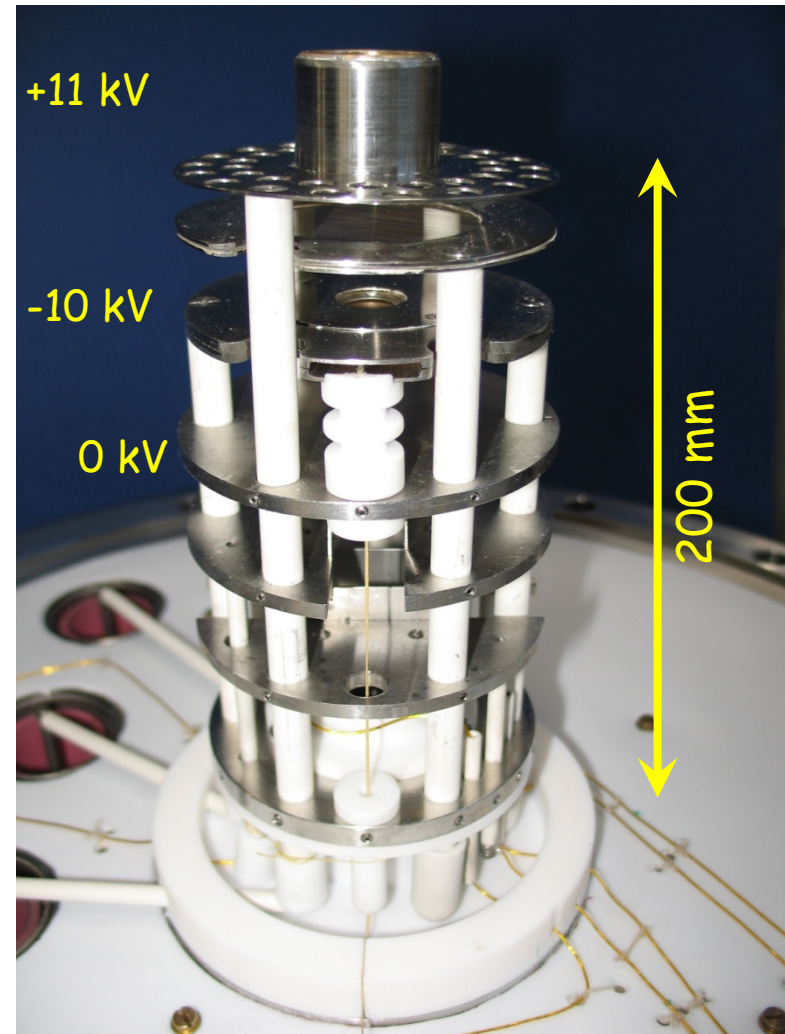
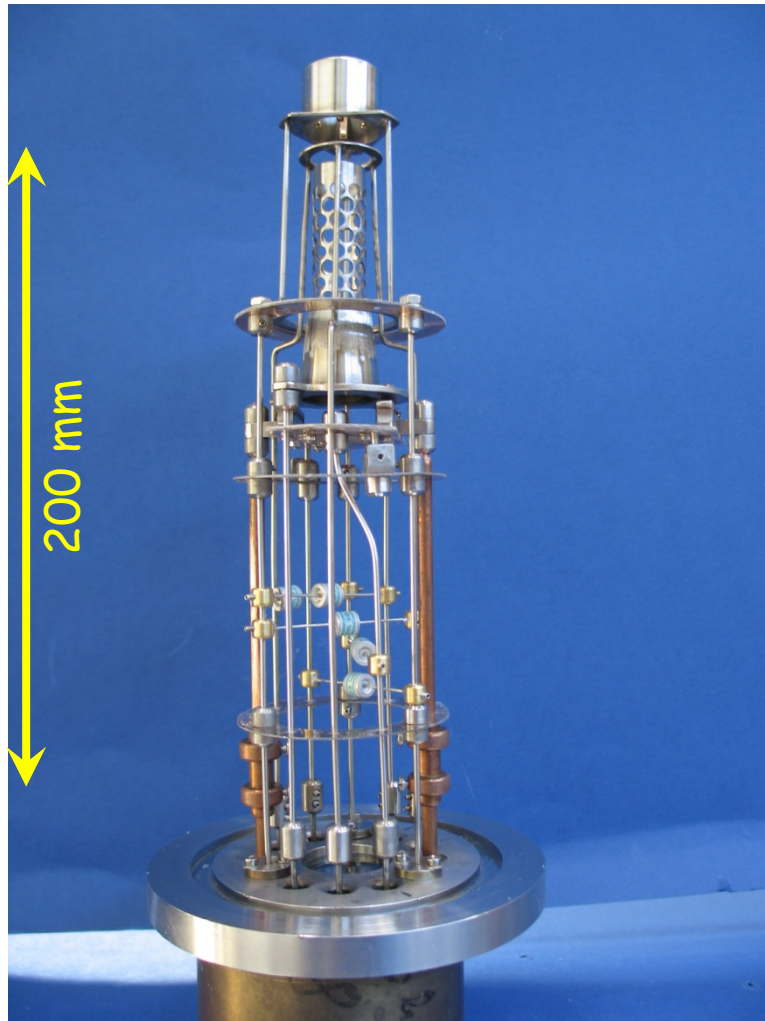


- SC wire NiTi+Cu (\varnothing 0.5 mm)
- Nominal current 50 A \Rightarrow $B \sim 1$ T
- Degradation of frozen field $\leq 0.1\%$ per 5 hrs
- LHe consumption ~ 8 l/h

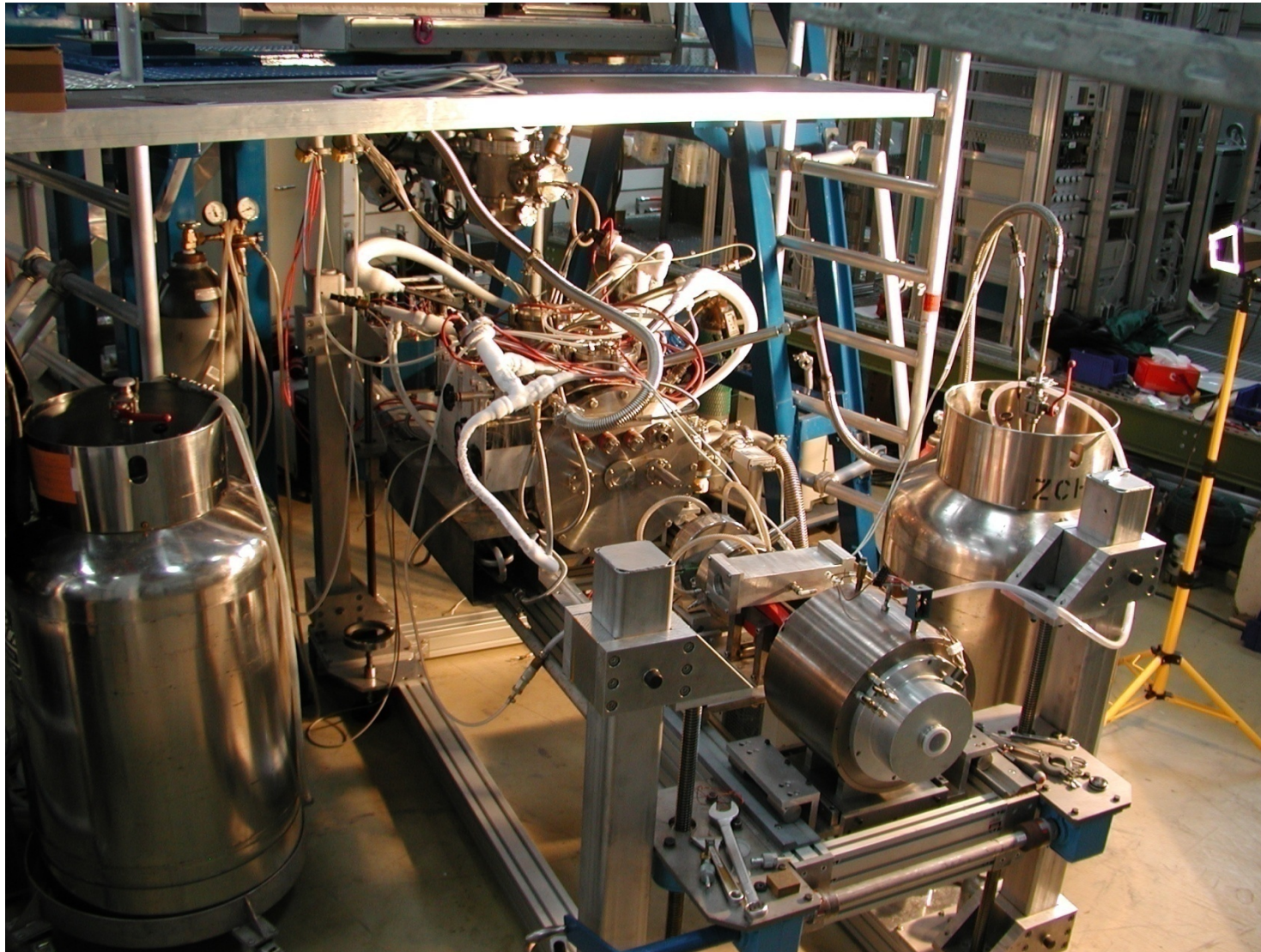


The experimental Setup

e^- -gun and ion optics



The experimental Setup



Important Details: H₂ Molecules

ortho-hydrogen	para-hydrogen
$ \uparrow\uparrow\rangle$	$\frac{1}{\sqrt{2}}(\uparrow\downarrow\rangle - \downarrow\uparrow\rangle)$
$\frac{1}{\sqrt{2}}(\uparrow\downarrow\rangle + \downarrow\uparrow\rangle)$	
$ \downarrow\downarrow\rangle$	

S=1

S=0

$\text{o-H}_2 \leftrightarrow \text{p-H}_2 \quad : \quad \Delta E = - 0.08 \text{ kJ/mol}$

$J = 1, 3, 5$

$J = 0, 2, 4$

$T \rightarrow 0 \text{ K:} \quad 0 \quad :$

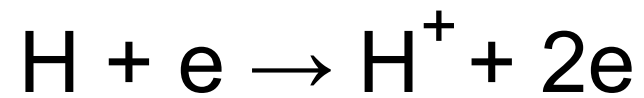
$T = 300 \text{ K:} \quad 3 \quad : \quad 1$

Polarized H₂ Molecules

$\Psi_{a,b}(I, m_I)$ and $I_a = 1, I_b = 1$
ortho-deuterium
$\Psi(2, 2) = \Psi_a(1, 1)\Psi_b(1, 1)$
$\Psi(2, 1) = \frac{1}{\sqrt{2}}[\Psi_a(1, 0)\Psi_b(1, 1) + \Psi_a(1, 1)\Psi_b(1, 0)]$
$\Psi(2, 0) = \frac{1}{\sqrt{6}}[\Psi_a(1, 1)\Psi_b(1, -1) + 2\Psi_a(1, 0)\Psi_b(1, 0) + \Psi_a(1, -1)\Psi_b(1, 1)]$
$\Psi(2, -1) = \frac{1}{\sqrt{2}}[\Psi_a(1, 0)\Psi_b(1, -1) + \Psi_a(1, -1)\Psi_b(1, 0)]$
$\Psi(2, -2) = \Psi_a(1, -1)\Psi_b(1, -1)$
$\Psi(0, 0) = \frac{1}{\sqrt{3}}[\Psi_a(1, 1)\Psi_b(1, -1) - \Psi_a(1, 0)\Psi_b(1, 0) + \Psi_a(1, -1)\Psi_b(1, 1)]$
para-deuterium
$\Psi(1, 1) = \frac{1}{\sqrt{2}}[\Psi_a(1, 1)\Psi_b(1, 0) - \Psi_a(1, 0)\Psi_b(1, 1)]$
$\Psi(1, 0) = \frac{1}{\sqrt{2}}[\Psi_a(1, +1)\Psi_b(1, -1) - \Psi_a(1, -1)\Psi_b(1, 1)]$
$\Psi(1, -1) = \frac{1}{\sqrt{2}}[\Psi_a(1, 0)\Psi_b(1, -1) - \Psi_a(1, -1)\Psi_b(1, 0)]$

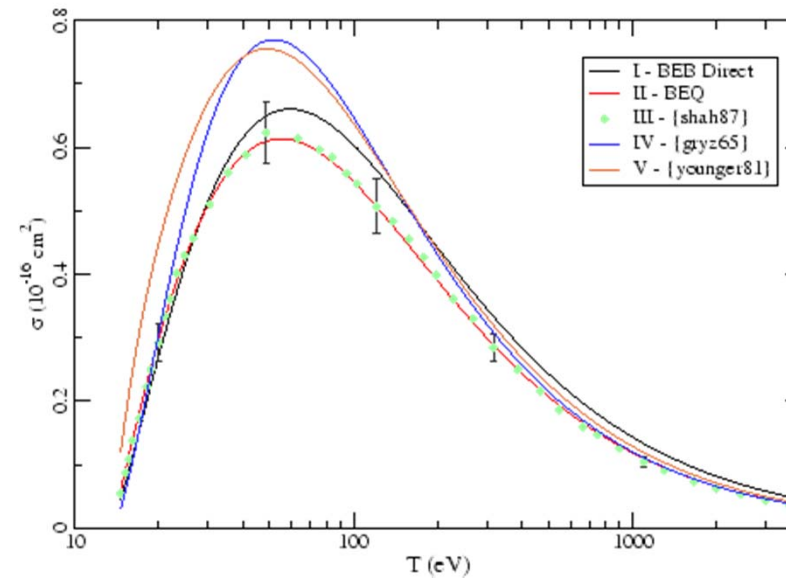
S=0 and S=2 are the groundstates

The Ionization Processes



($E_e = 150 \text{ eV}$: $\sigma = 0.46 \cdot 10^{-16} \text{ cm}^2$)

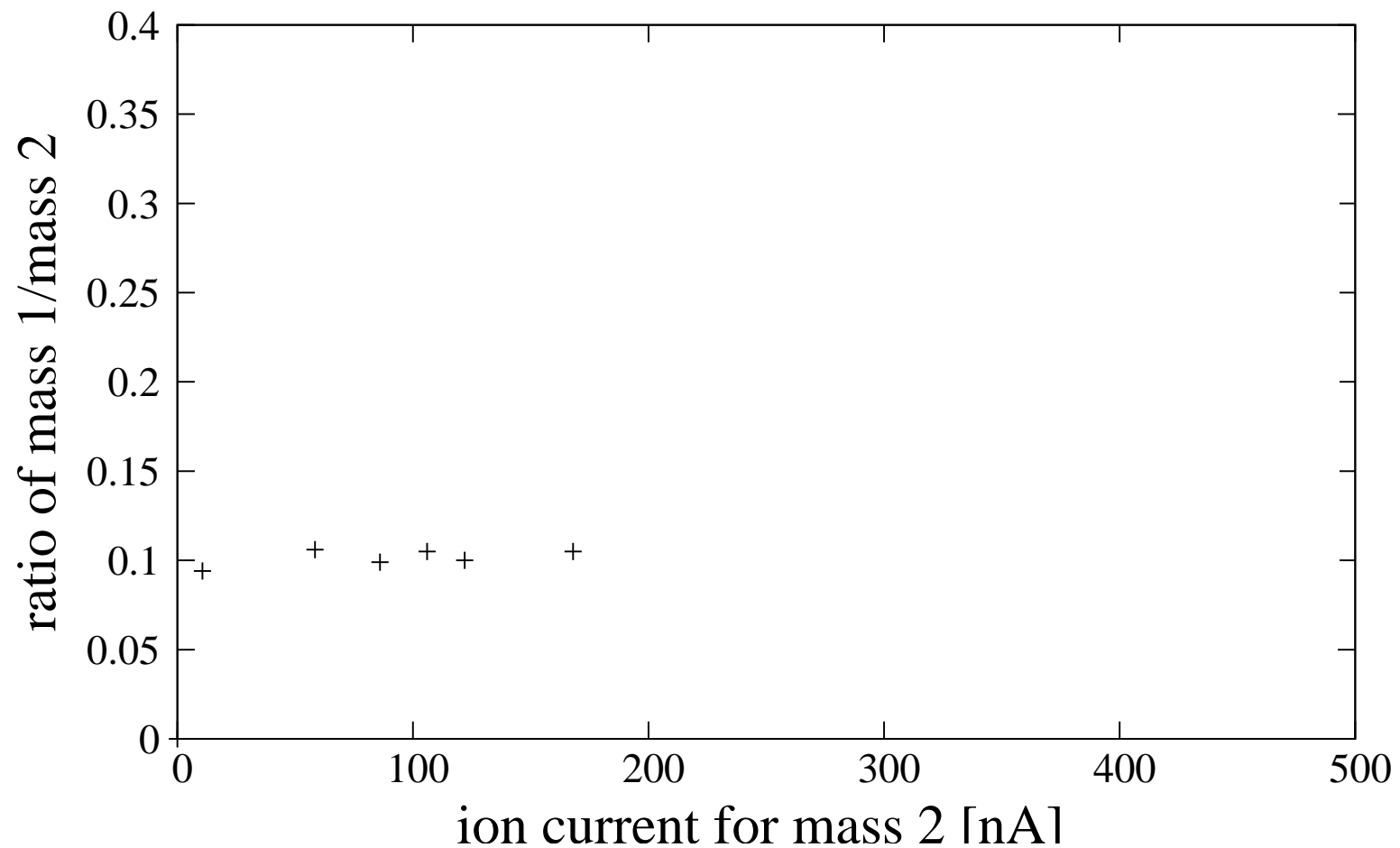
Neutral Hydrogen Total Ionization Cross-Section



(www.nist.gov)

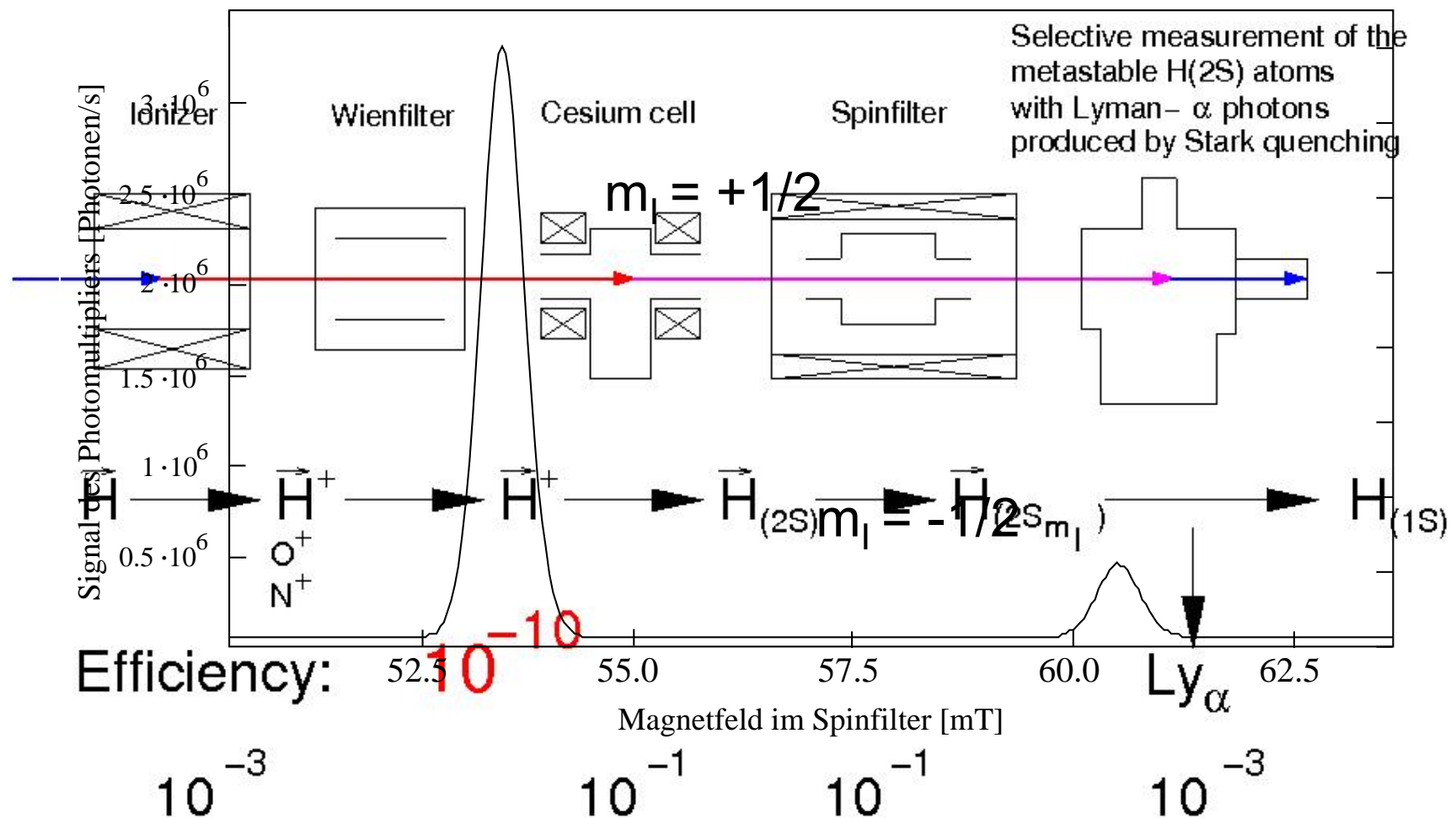
Recombination

Storage cell filled with H₂ gas with different fluxes

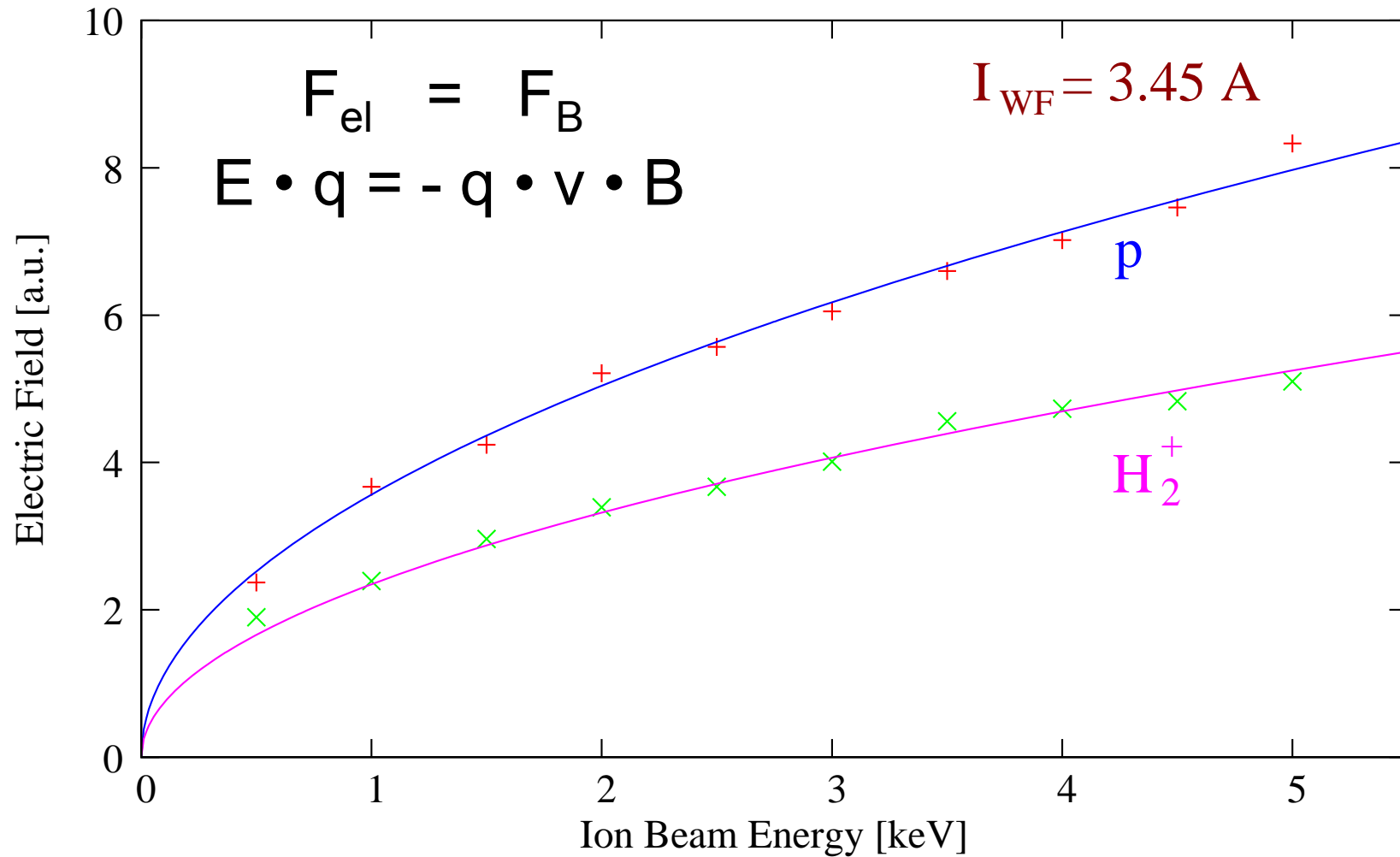


The experimental Setup

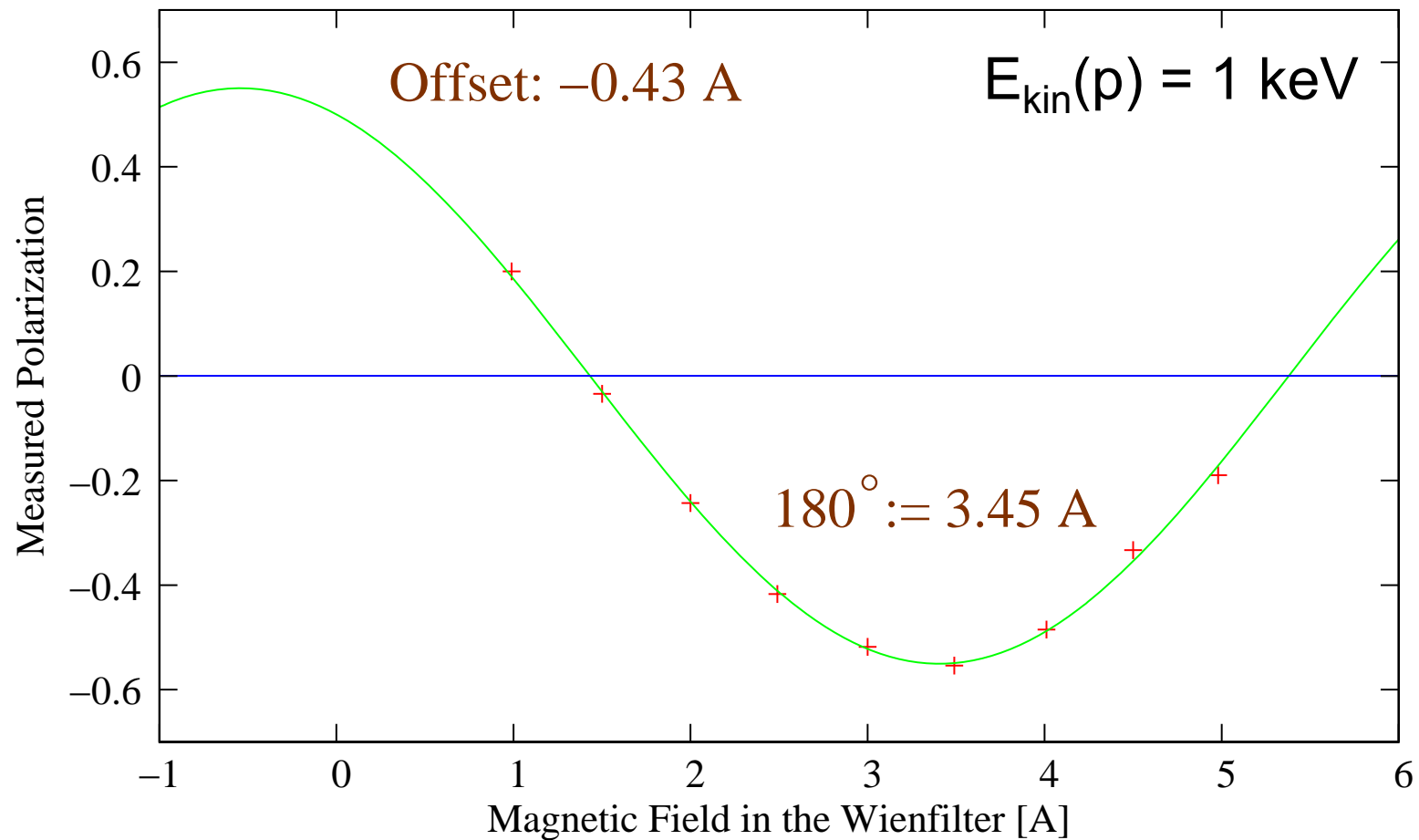
The Lamb-shift Polarimeter



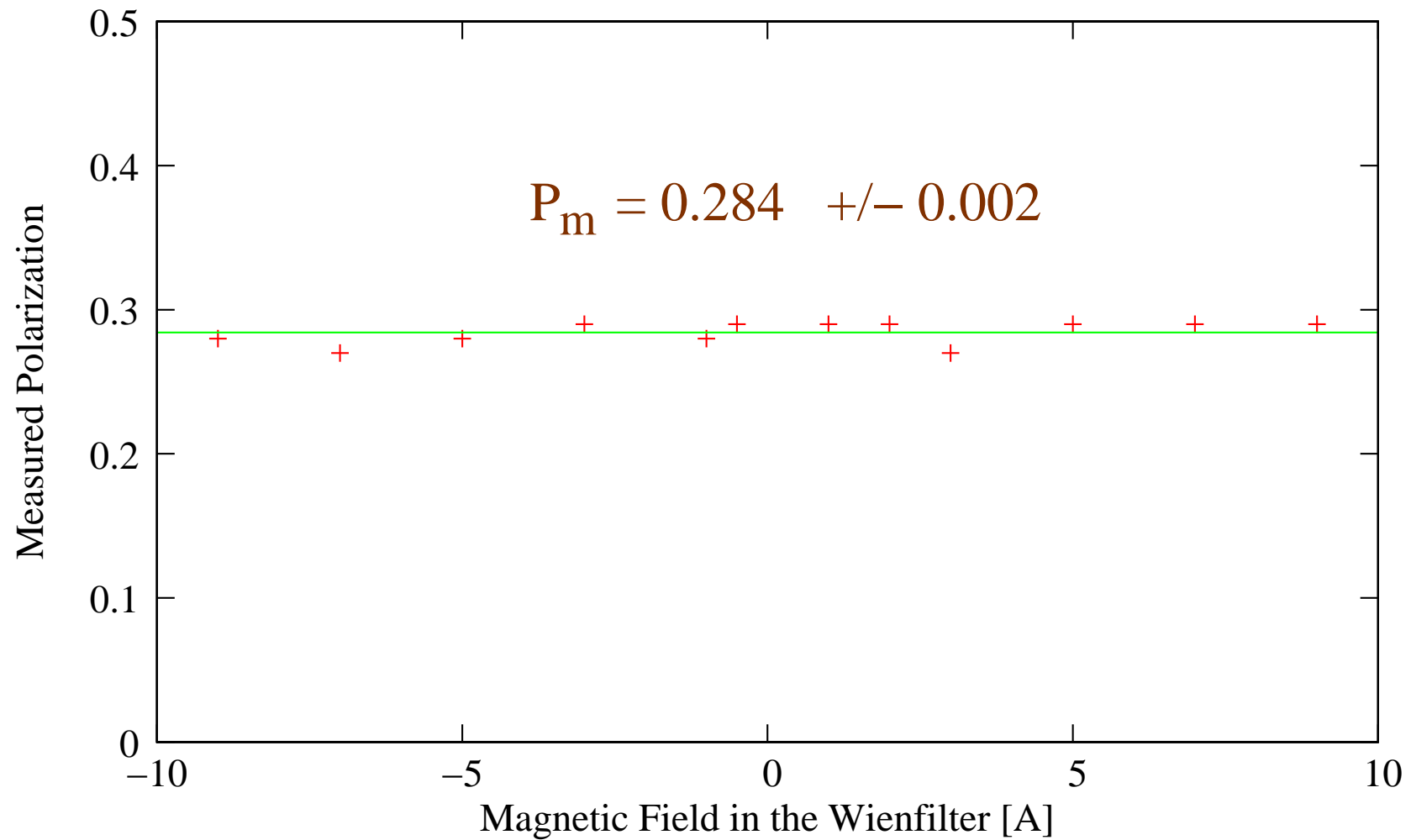
Mass separation with the Wienfilter



Wienfilter function of the protons in the LSP



Experimental results



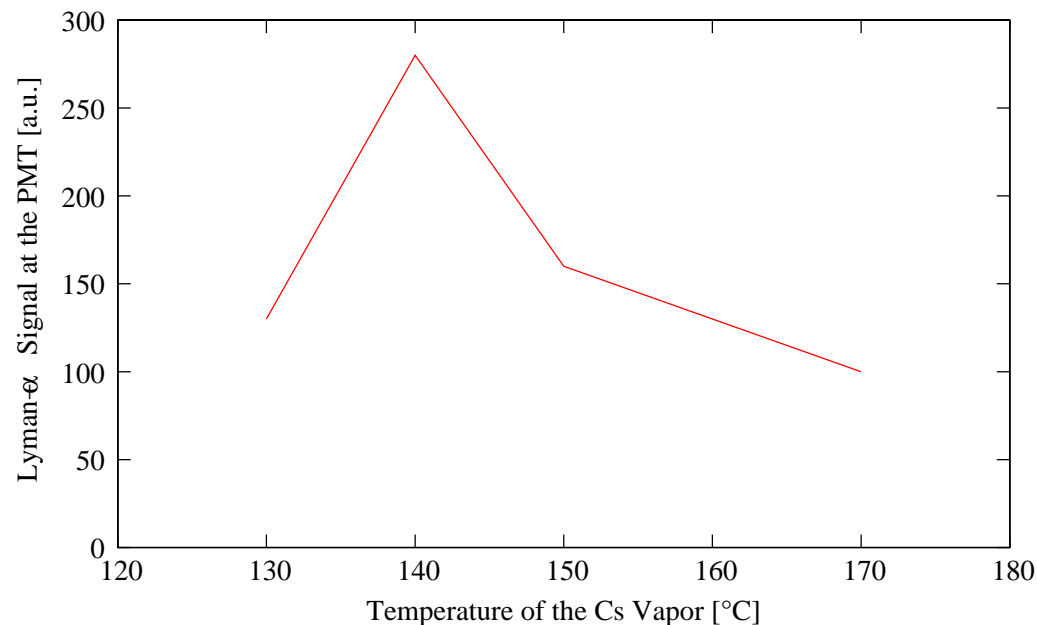
Experimental results

How are the polarized $\text{H}_{2\text{S}}$ produced from H_2^+ ?

2-step process (Stripping at the Cs + $\text{H}_{2\text{S}}$ production)



1-step process: Direct production: $\text{H}_2^+ + \text{Cs} \rightarrow \text{H}_{2\text{S}} + \text{Cs}^+ \dots$



Cross section:
 $\sigma(p \rightarrow \text{H}_{2\text{S}}) \approx 35 \cdot \sigma(\text{H}_2^+ \rightarrow \text{H}_{2\text{S}})$

R. Engels et al.;
 Rev. Sci. Instr. **85** (2014)103505

Polarization losses of the molecules

A. Abragam: The Principles of Nuclear Magnetism (1961)

Spin Relaxation of H₂/D₂ Molecules

- The polarization losses during wall collision depend on:
- Nuclear Spin I
 - Polarization P_m
 - Temperature
 - Magnetic field in the cell

A. Abragam: The Principles of Nuclear Magnetism

Hamiltonian to describe the nuclear relaxation of a H_2 molecules

$$H = \omega_I (I_z^1 + I_z^2) + \omega_J J_z + \omega' (I^1 + I^2) \cdot J + \omega'' \{ I^1 \cdot I^2 - 3(I^1 \cdot n)(I^2 \cdot n) \}$$

I^1 and I^2 are the spins of the two protons

$$I^1 + I^2 = I$$

J is the rotational angular momentum of the molecule

$\omega_I = -\gamma_I H_0$ is the proton Lamor frequency in the applied field H_0

$\omega_J = -\gamma_J H_0$ is the Lamor frequency of the rotational magnetic moment of the H_2

$\omega' = -\gamma_I H'$ is the strength of the coupling between the magnetic moment of the protons and the magnetic field produced at their positions by the rotation of the molecule ($H' = 2.7$ mT)

$\omega'' = 2 \gamma_I H'' = \gamma_I^2 \hbar / b^3$ is the strength of the dipolar coupling between the protons, b is their distance, and n is the unit vector b/b ($H'' = 3.4$ mT).

Polarization losses of the molecules

A. Abragam: The Principles of Nuclear Magnetism (1961)

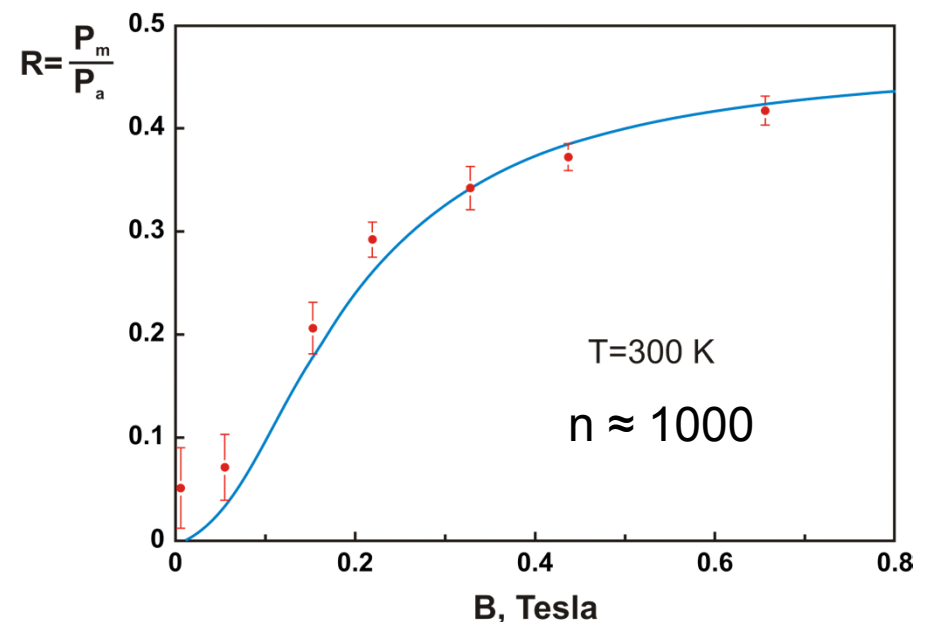
Spin Relaxation of H₂/D₂ Molecules

→ The polarization losses during wall collision depend on:

- Nuclear Spin I
- Polarization P_m
- Temperature
- Magnetic field in the cell

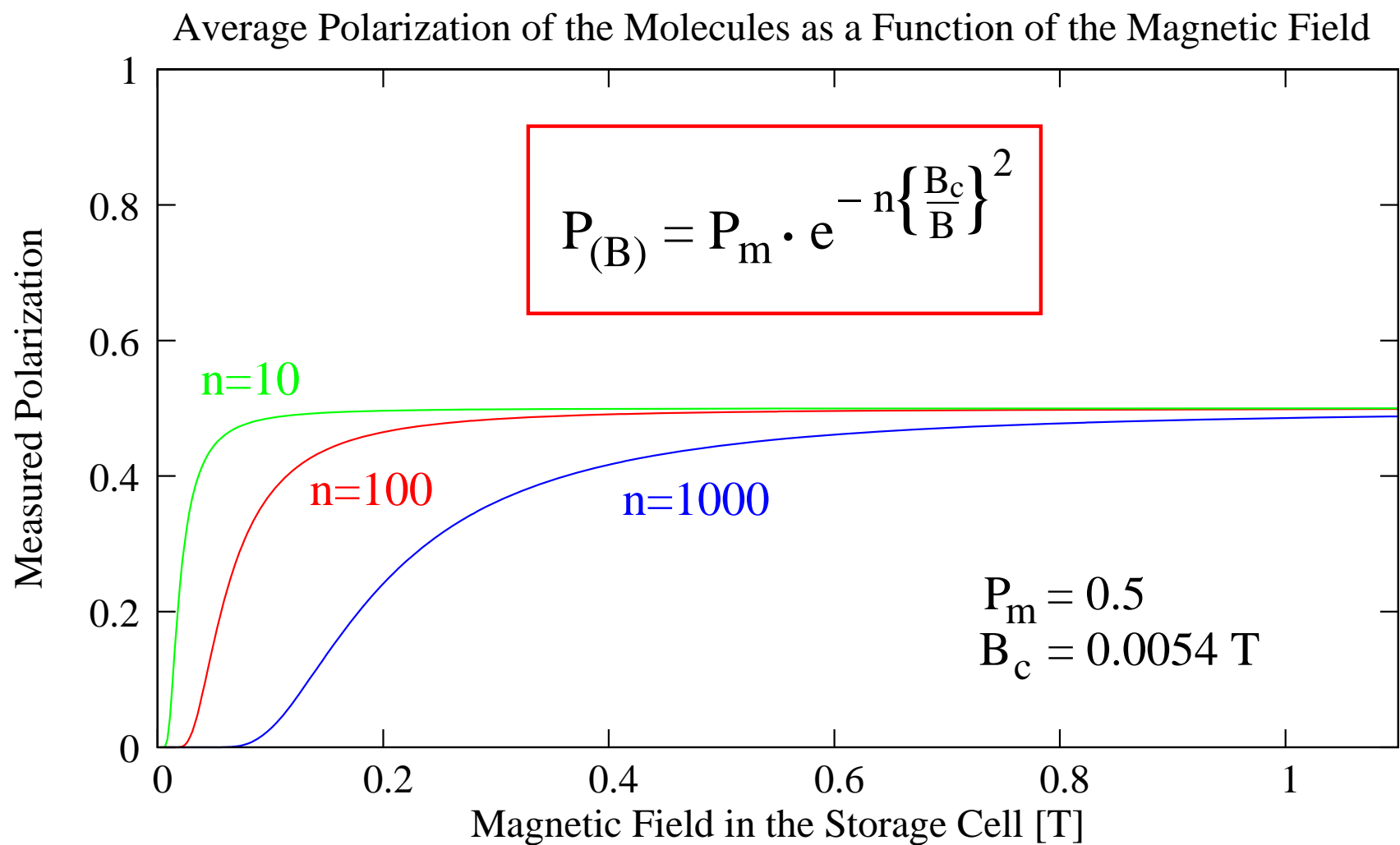
$$P_{(B,n)} = P_m \cdot e^{-n \left(\frac{B_c}{B} \right)^2}$$

→ $B_c = 5.4 \text{ mT}$
(For $T \sim 100 \text{ K}$)

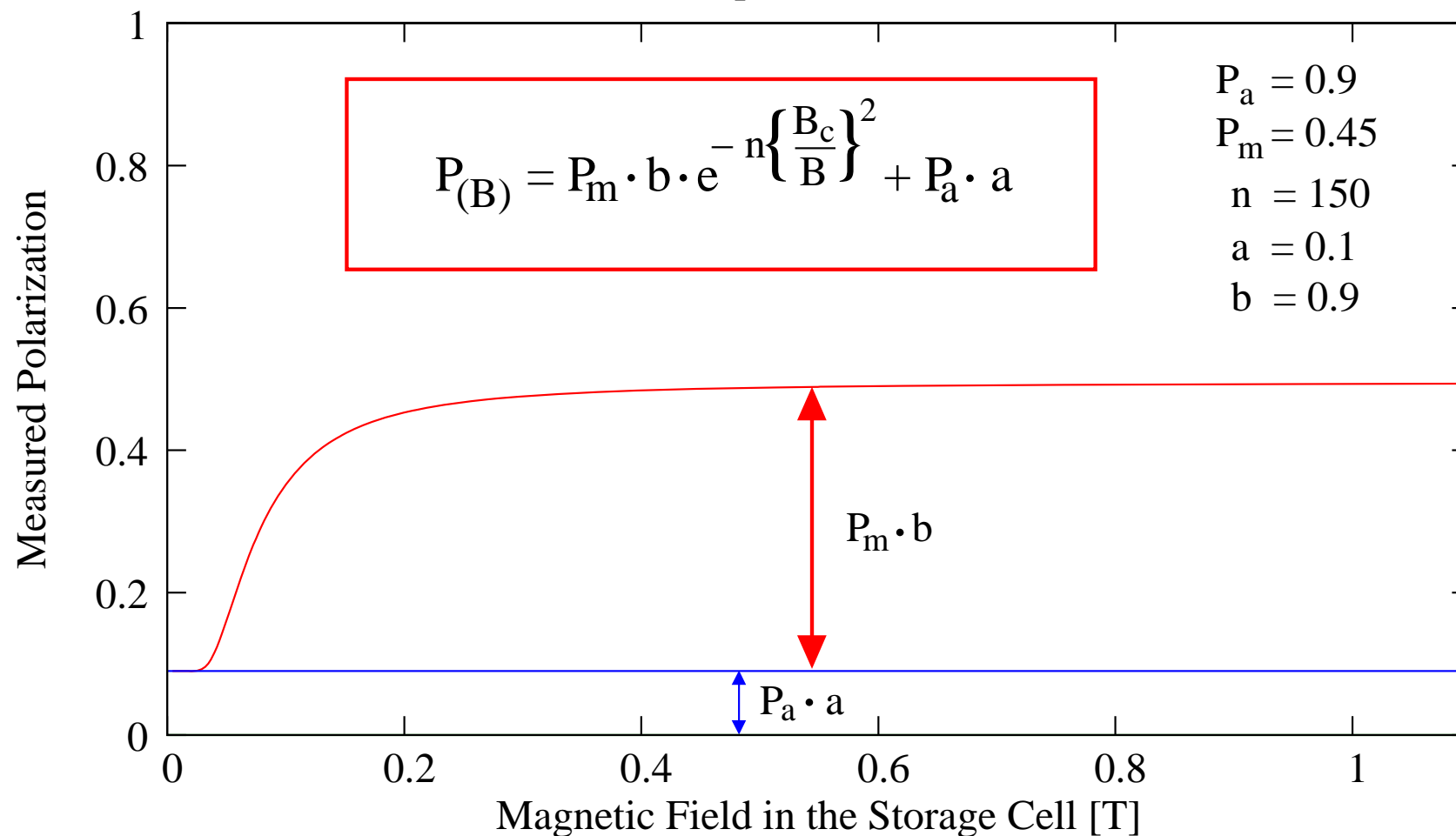


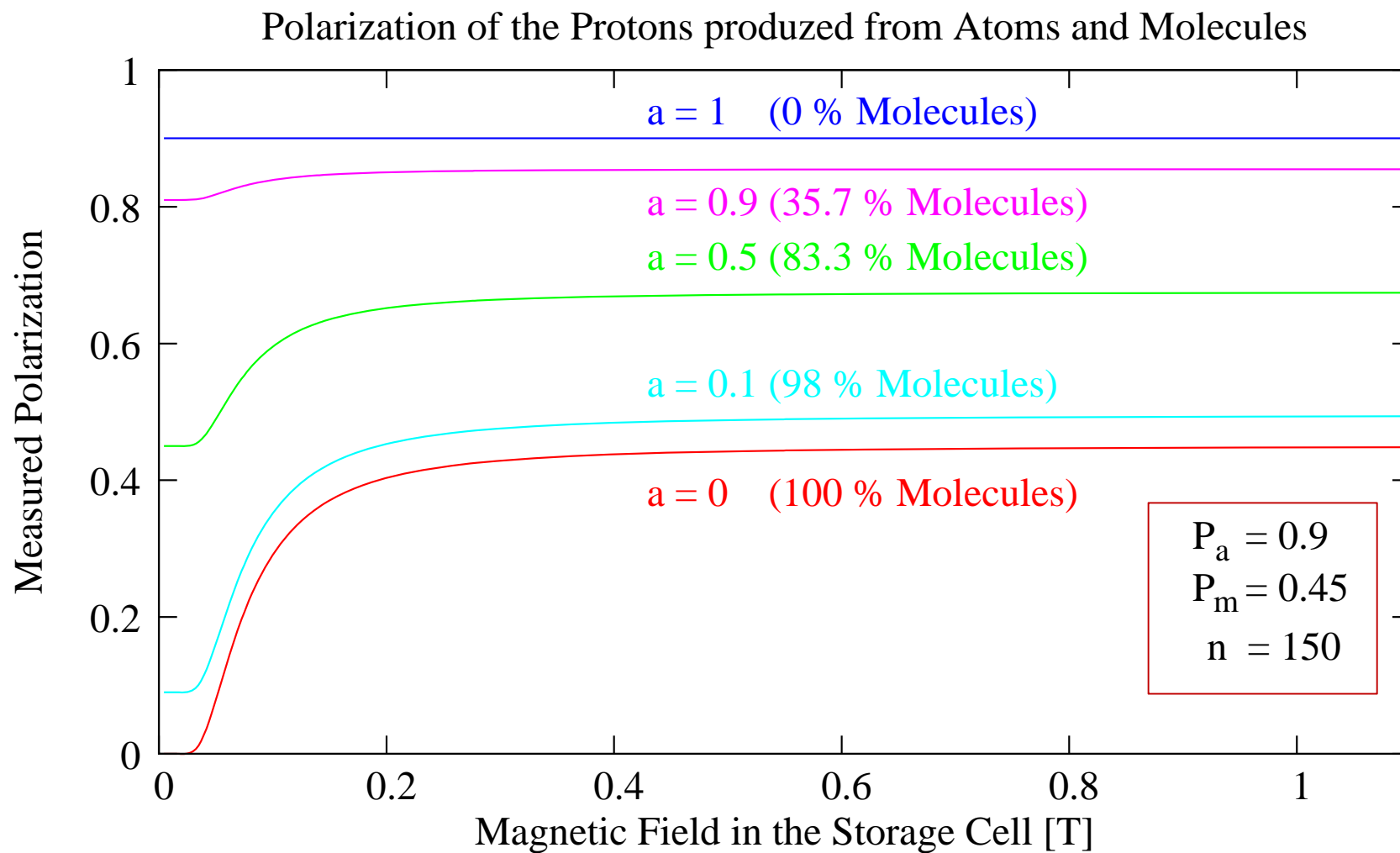
Nuclear Polarization of Hydrogen Molecules from
Recombination of Polarized Atoms
T.Wise et al., Phys. Rev. Lett. 87, 042701 (2001).

$$\lim_{B \rightarrow \infty} R = 0.5$$

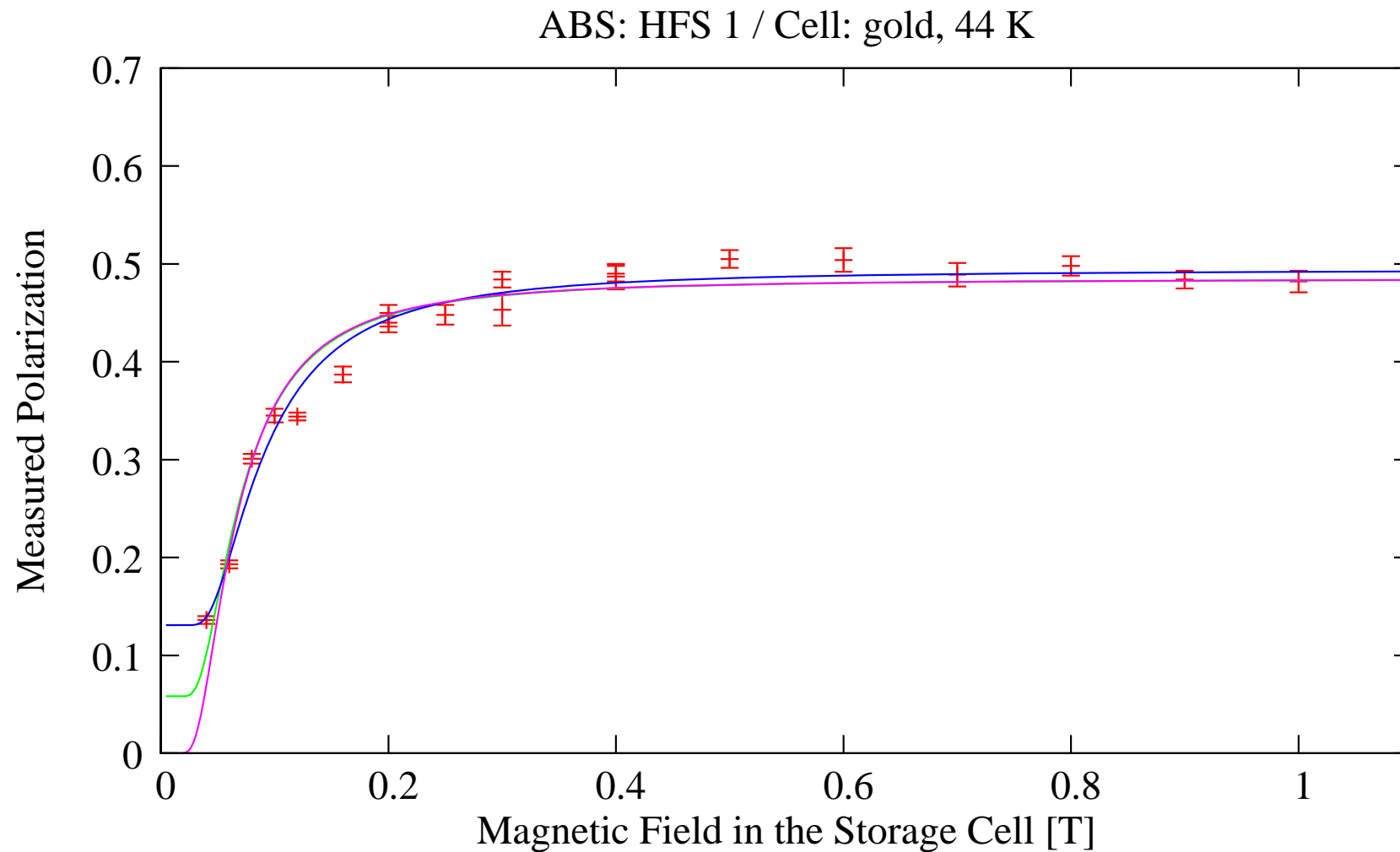


Polarization of the Protons produced from Atoms and Molecules





Experimental results: Polarization of Protons



n can have different distributions $W(n)$!

Simplest Case (cylindrical geometries / elastic scattering):

$$\rightarrow W_{(n)} = 1/\alpha \ e^{-\alpha n}$$

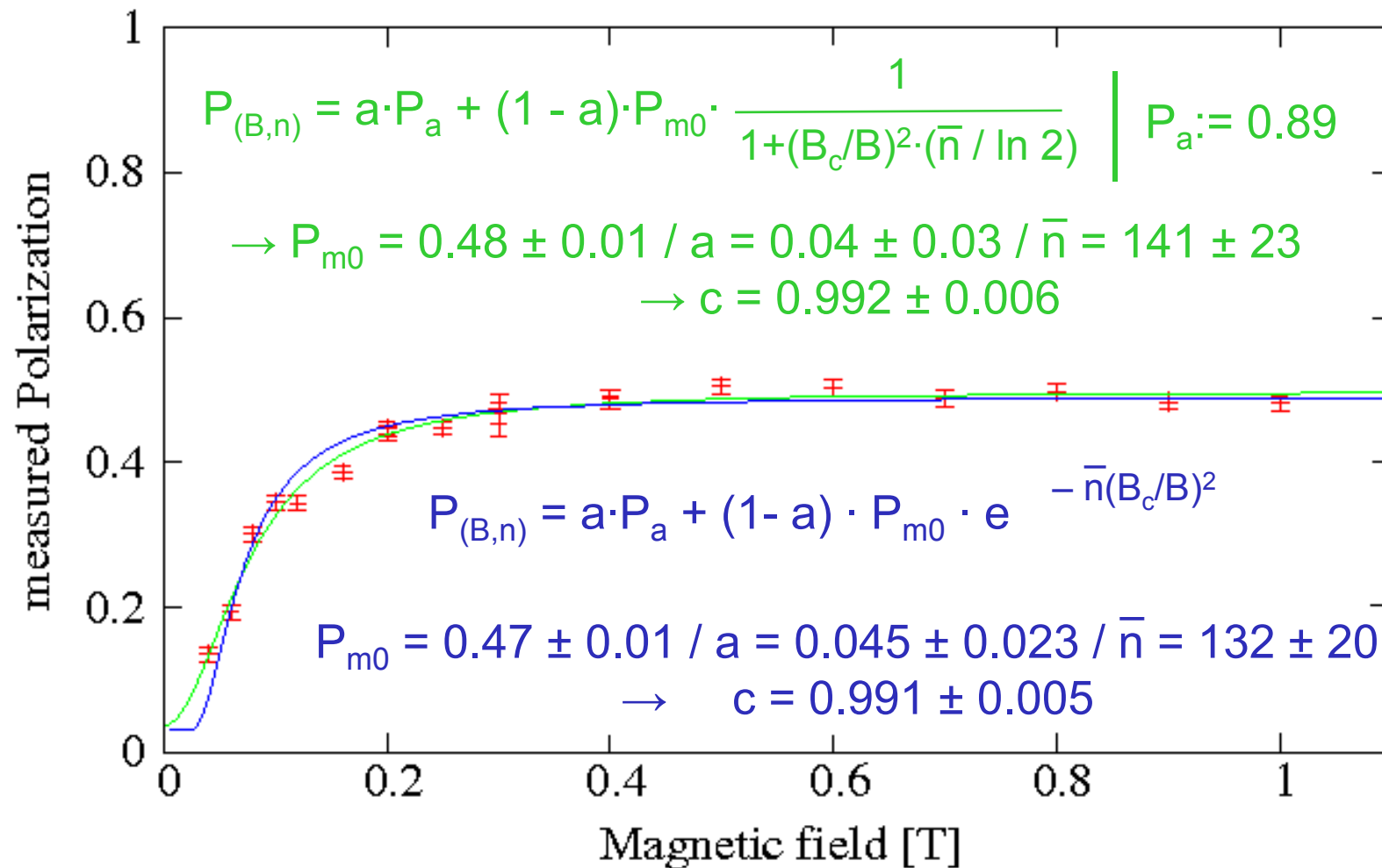
$$\rightarrow \bar{n} = \ln 2 / \alpha$$

$$\rightarrow P_m(B, n) = P_{m_0} \cdot \frac{1}{1 + (B_c/B)^2 \cdot \bar{n} / \ln 2}$$

More complicated cases (e.g. $\cos^{0,1,2, \dots}$ distribution of the molecules, when they are leaving the surface) deliver different $W(n)$ and \bar{n} .

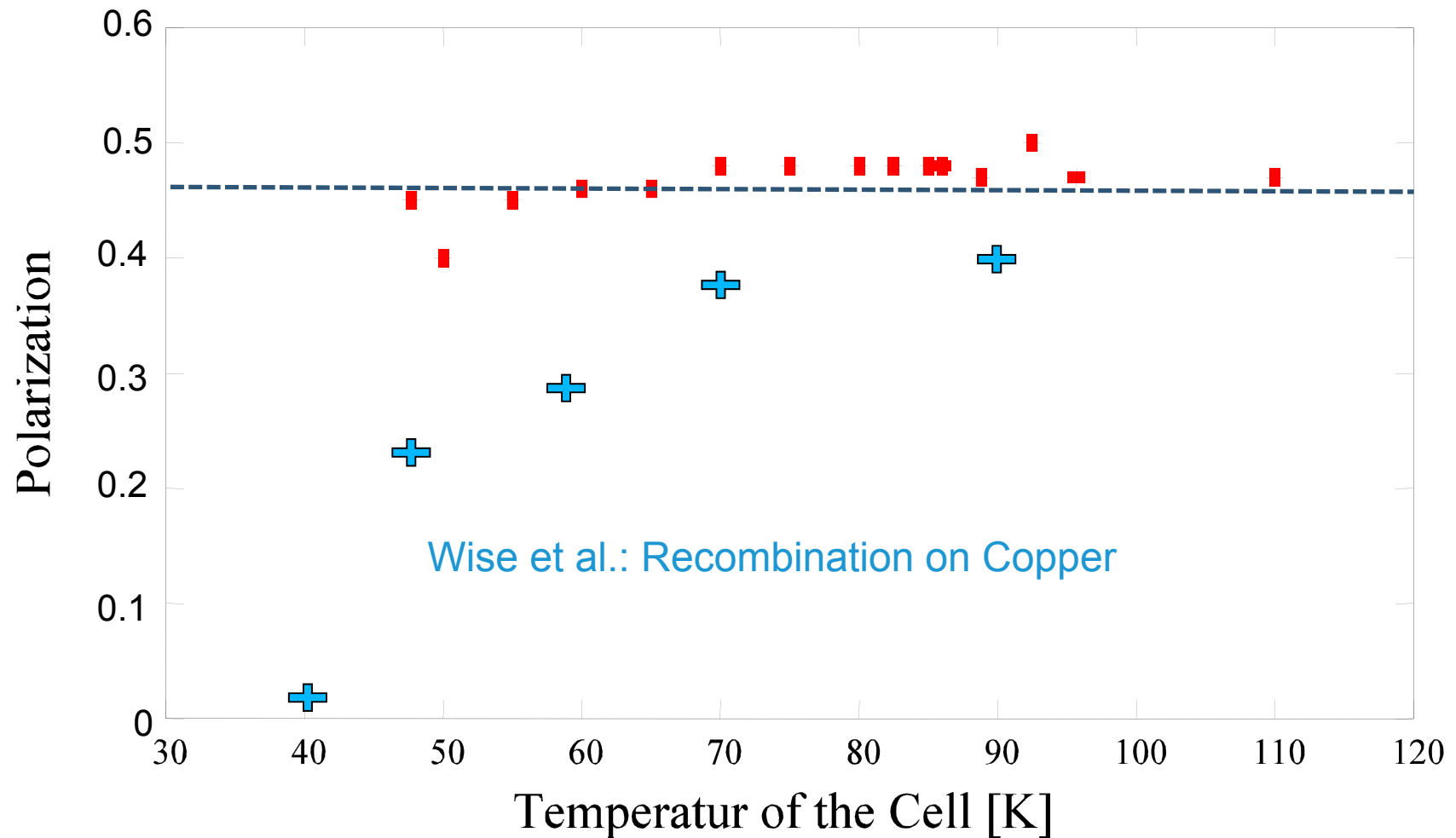
Experimental results: Polarization of Protons

HFS 1 $\rightarrow P_a = 0.89$ / Temperature: 44 K



Experimental results

Polarization of Hydrogen Molecules and Atoms
(Surface: Gold, HFS 1, $B = 0.28$ T, $Q = 4$ keV)



Experimental results

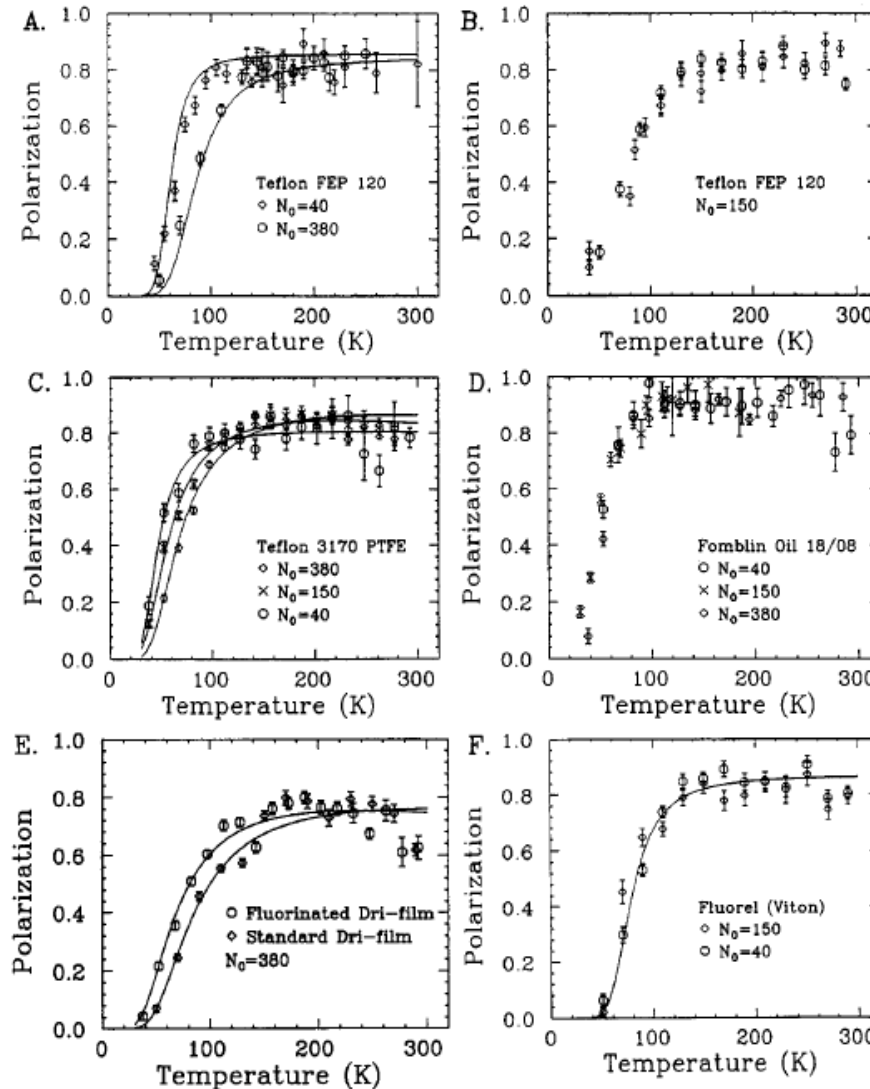


Fig. 4. Measured \bar{H}^0 target polarization vs. cell wall temperature for Teflon, Fomblin, Dri-film and Viton coated onto 6061 aluminum cells. Polarization is expressed as a fraction of the expected maximum assuming no depolarization. N_0 is the average age of the target atoms in number of wall collisions. The solid lines are curves fit to the data as described in Section 7.

J.S. Price and W. Haeberli,

“Measurement of cell wall depolarization of polarized hydrogen gas targets in a weak magnetic field”

Nuclear Instruments and Methods in Physics Research A **349** (1994) 321-333

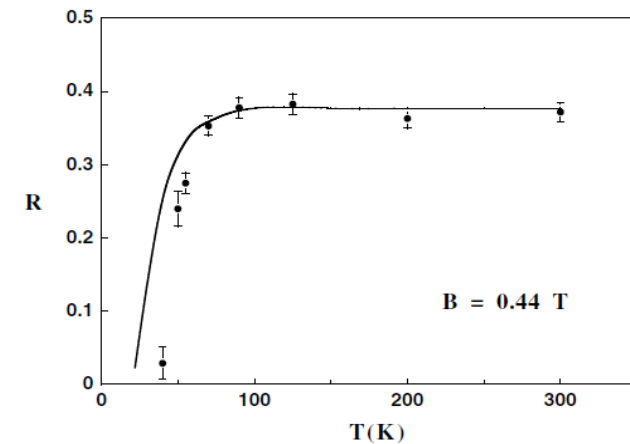
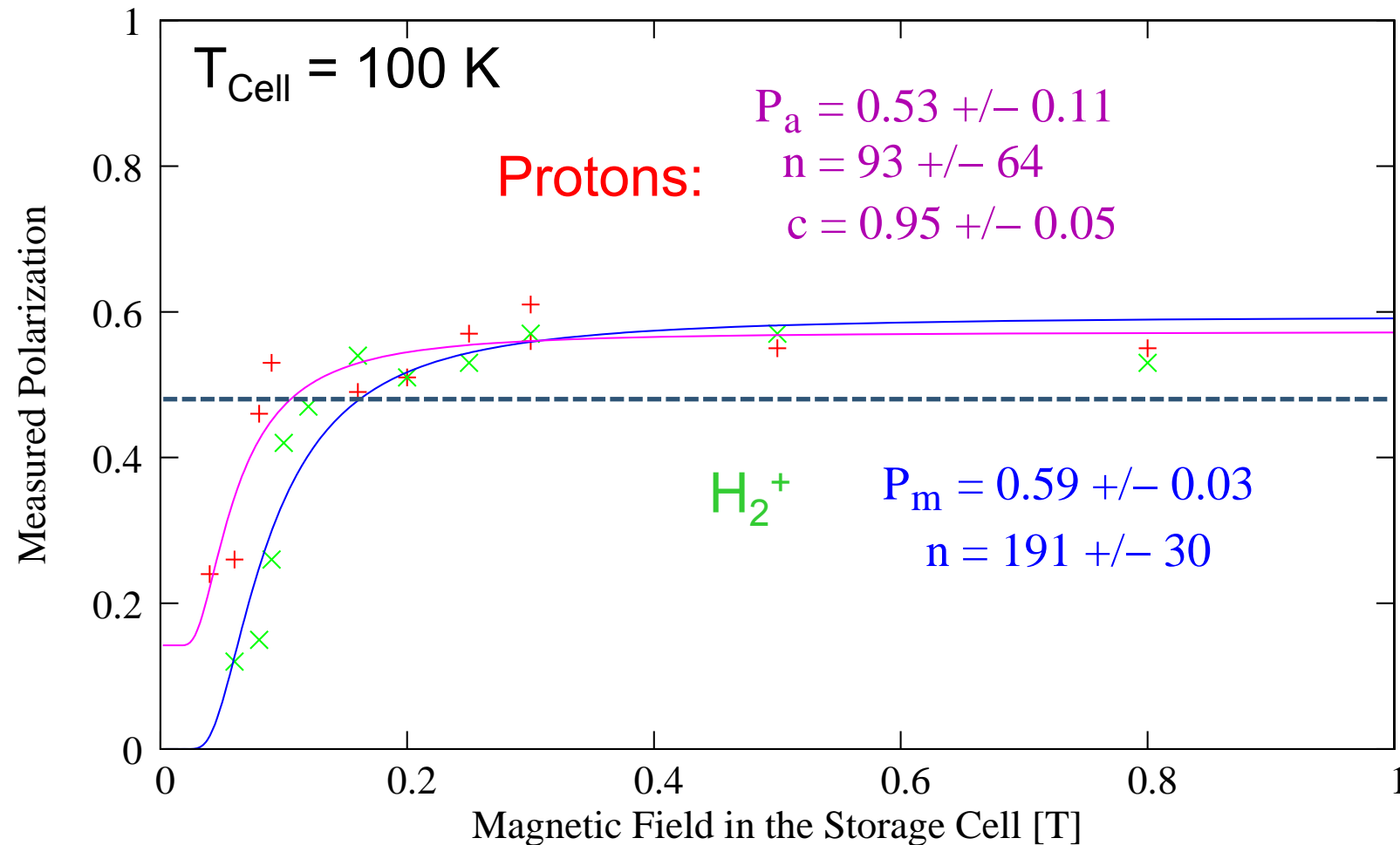


FIG. 3. Fraction R of proton polarization of the H atoms that is retained in the H_2 molecules after recombination on a copper surface at different temperatures T for a fixed magnetic field strength $B = 0.44$ T. The curve is based on measurements of the polarization of hydrogen atoms in a Cu cell in which about 65% of the atoms recombined; see Ref. [15].

Experimental results

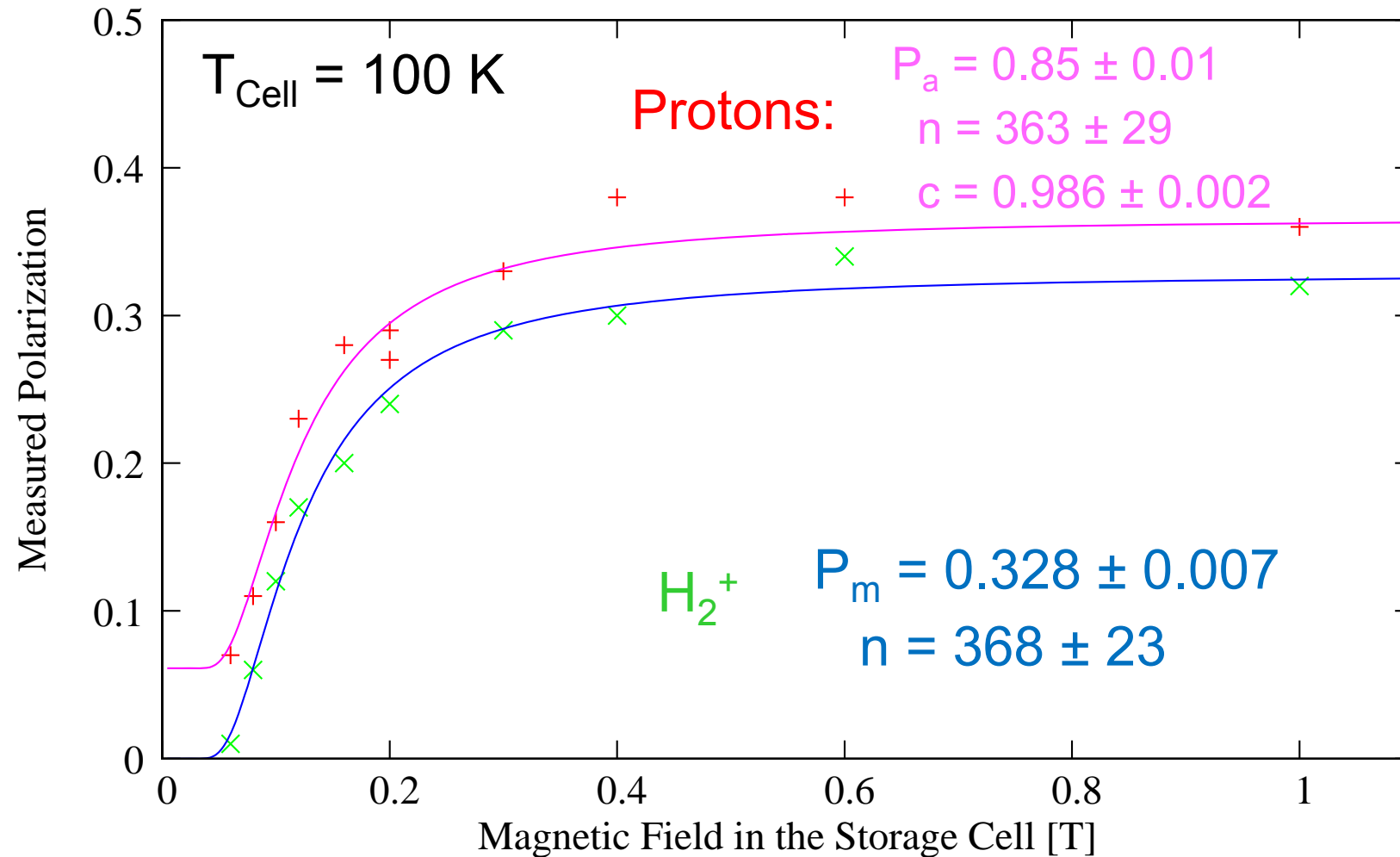
Measurements on Fused Quartz Glass in the first hours



$P_m = 66 \%$ of the original atomic Polarization

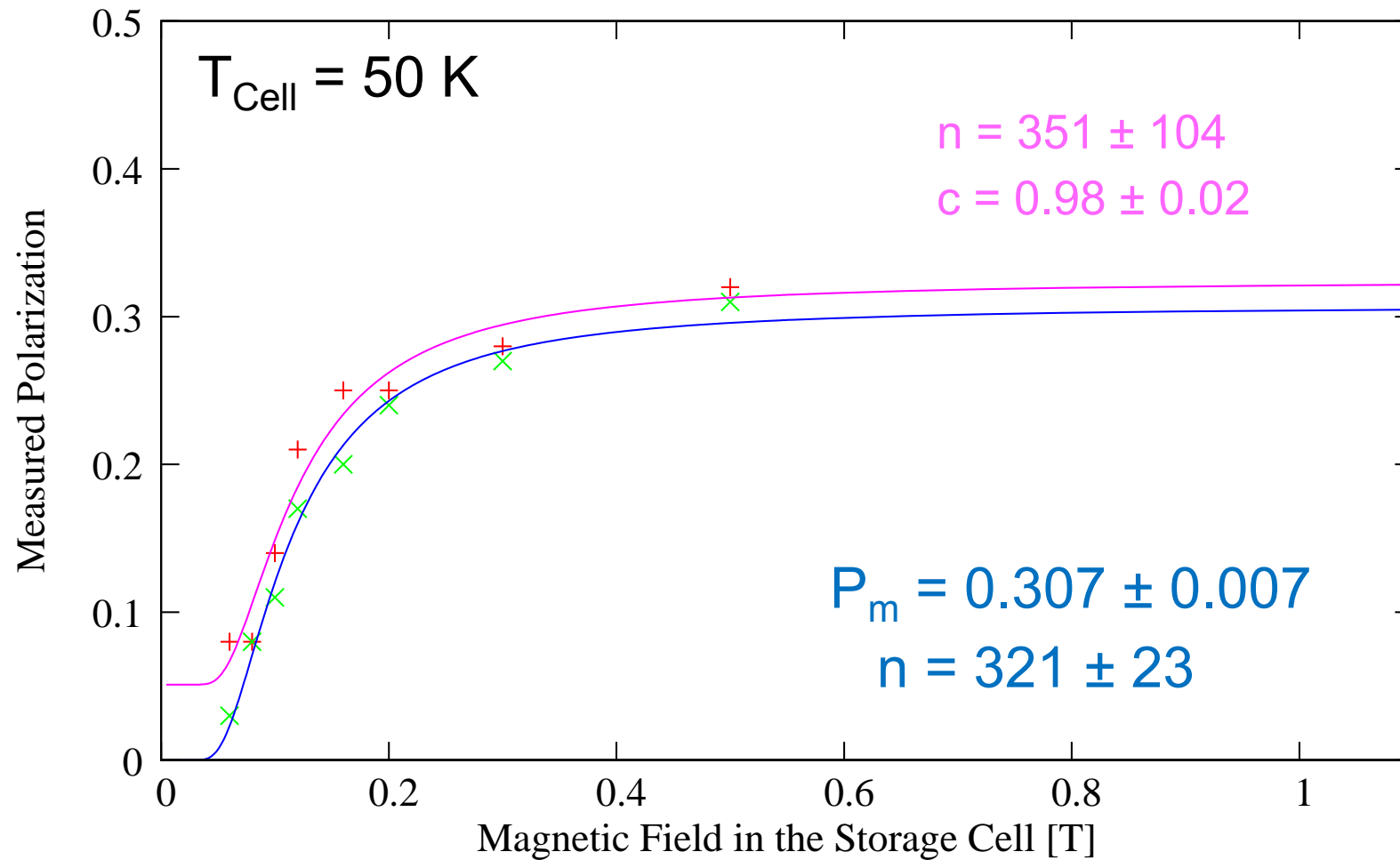
Experimental results

Measurements on Fused Quartz Glass after several days



Experimental results

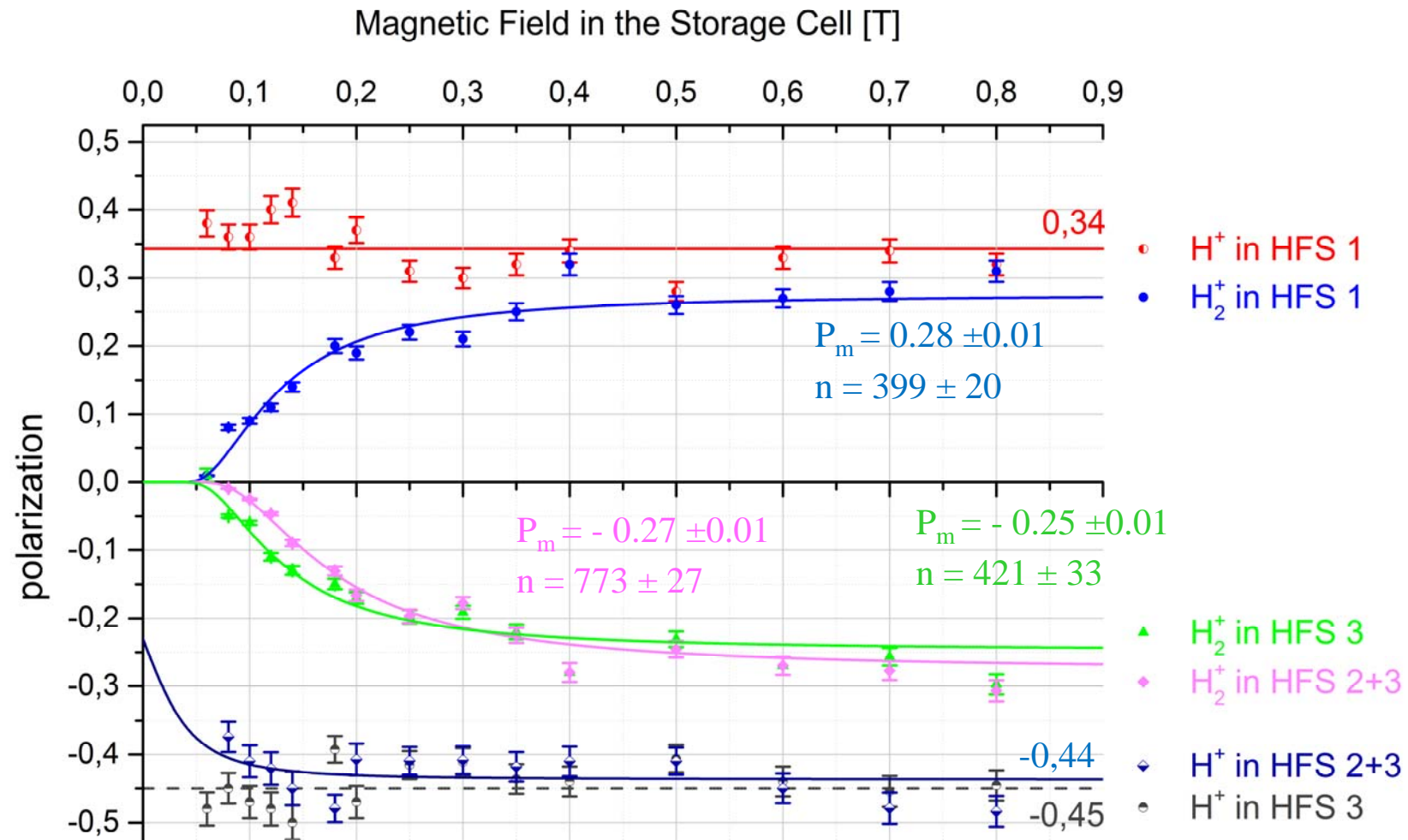
Measurements on Fused Quartz Glass after several days



No real changes between 50 and 100 K

Experimental results

Very first results on water: $T_{\text{cell}} = 100$ K (on fused quartz)

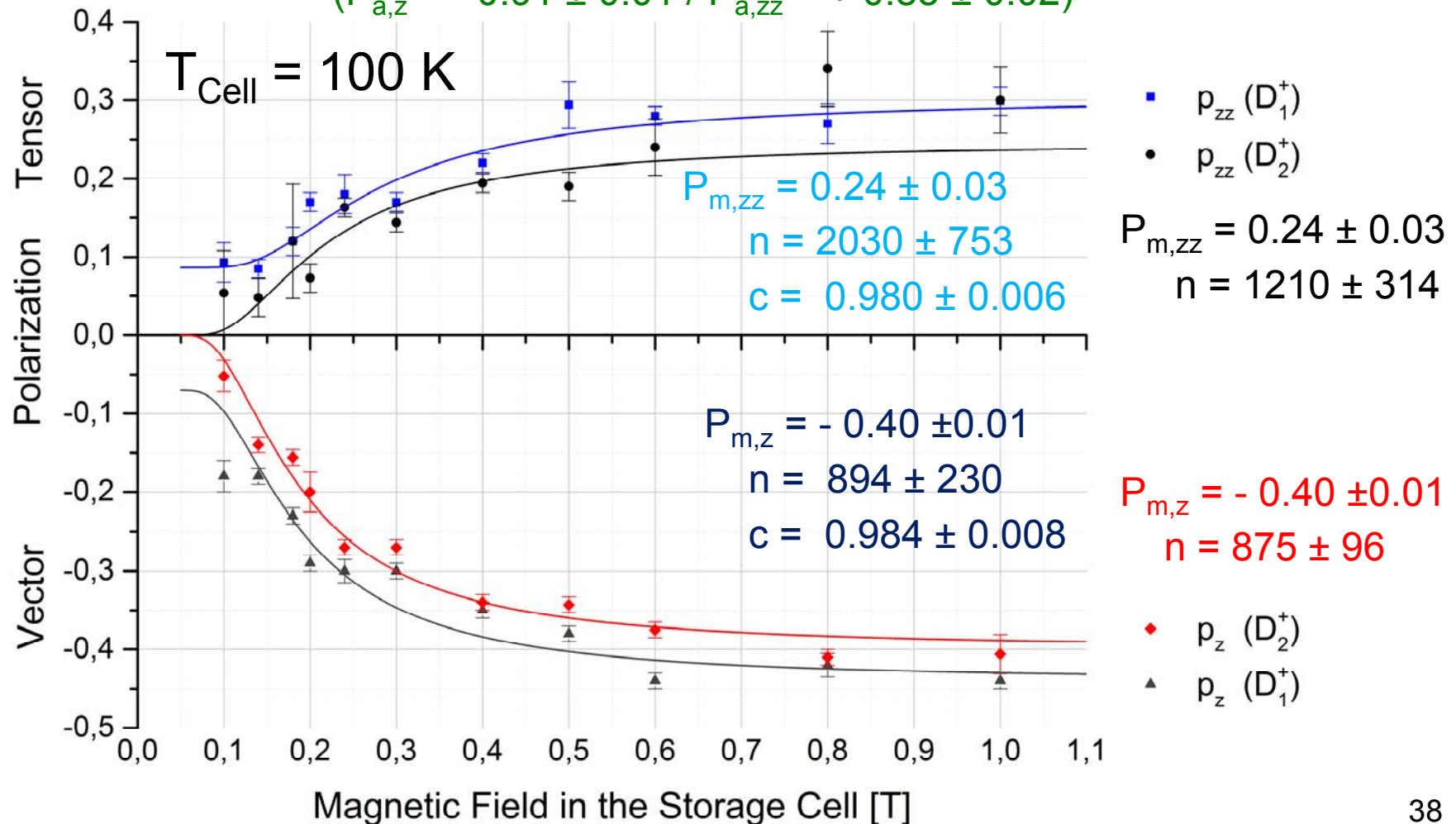


Experimental results

Measurements on Fused Quartz Glass after several days

Deuterium: HFS 3+4 (Vector and Tensorpolarized)

$$(P_{a,z} = -0.91 \pm 0.01 / P_{a,zz} = +0.85 \pm 0.02)$$



A. Abragam: The Principles of Nuclear Magnetism

Hamiltonian to describe the nuclear relaxation of a H_2 molecules

$$H = \omega_I (I_z^1 + I_z^2) + \omega_J J_z + \omega' (I^1 + I^2) \cdot J + \omega'' \{ I^1 \cdot I^2 - 3(I^1 \cdot n)(I^2 \cdot n) \}$$

I^1 and I^2 are the spins of the two protons

$$I^1 + I^2 = I$$

J is the rotational angular momentum of the molecule

$\omega_I = -\gamma_I H_0$ is the proton Larmor frequency in the applied field H_0

$\omega_J = -\gamma_J H_0$ is the Larmor frequency of the rotational magnetic moment of the H_2

$\omega' = -\gamma_I H'$ is the strength of the coupling between the magnetic moment of the protons and the magnetic field produced at their positions by the rotation of the molecule ($H' = 2.7$ mT)

$\omega'' = 2 \gamma_I H'' = \gamma_I^2 \hbar / b^3$ is the strength of the dipolar coupling between the protons, b is their distance, and n is the unit vector b/b ($H'' = 3.4$ mT).

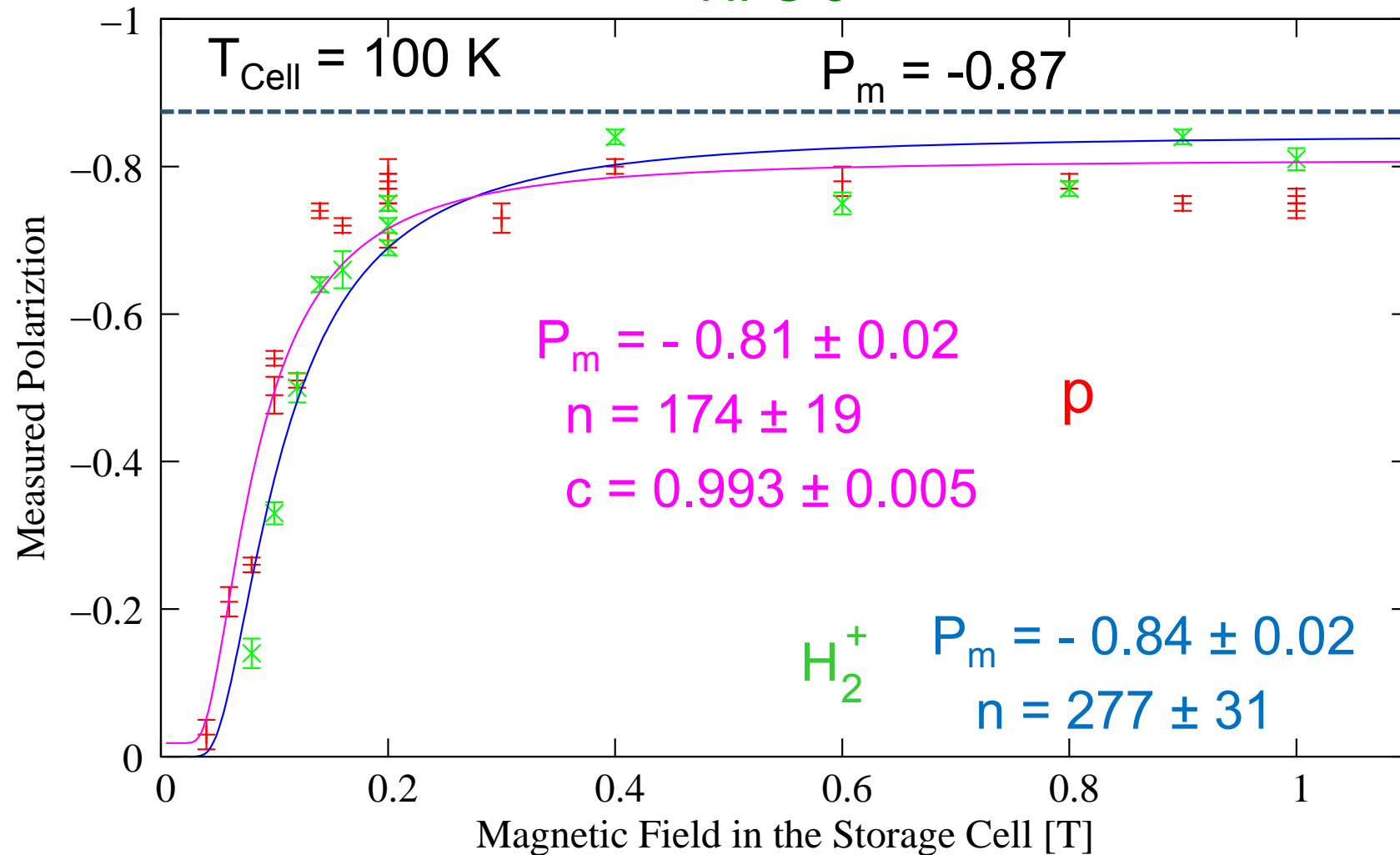
$$B_c(H_z) \neq B_c(D_z) \neq B_c(D_{zz})$$

$$\Rightarrow B_c(D_z) = 8 \pm 1 \text{ mT} / B_c(D_{zz}) = 11 \pm 1 \text{ mT}$$

Experimental results

Measurements on Fomblin Oil (Perfluoropolyether PFPE)

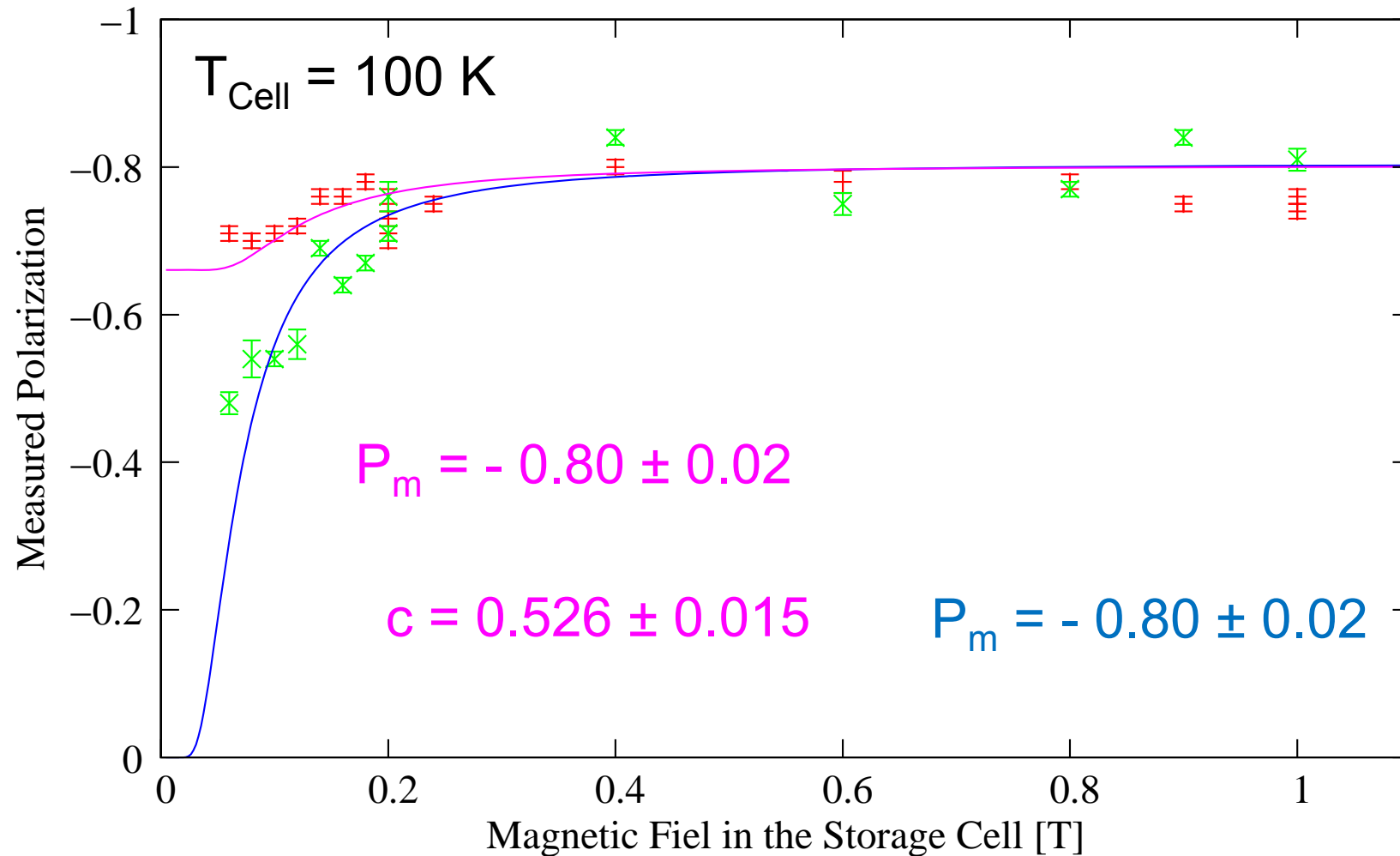
HFS 3



Experimental results

Measurements on Fomblin Oil (Perfluoropolyether PFPE)

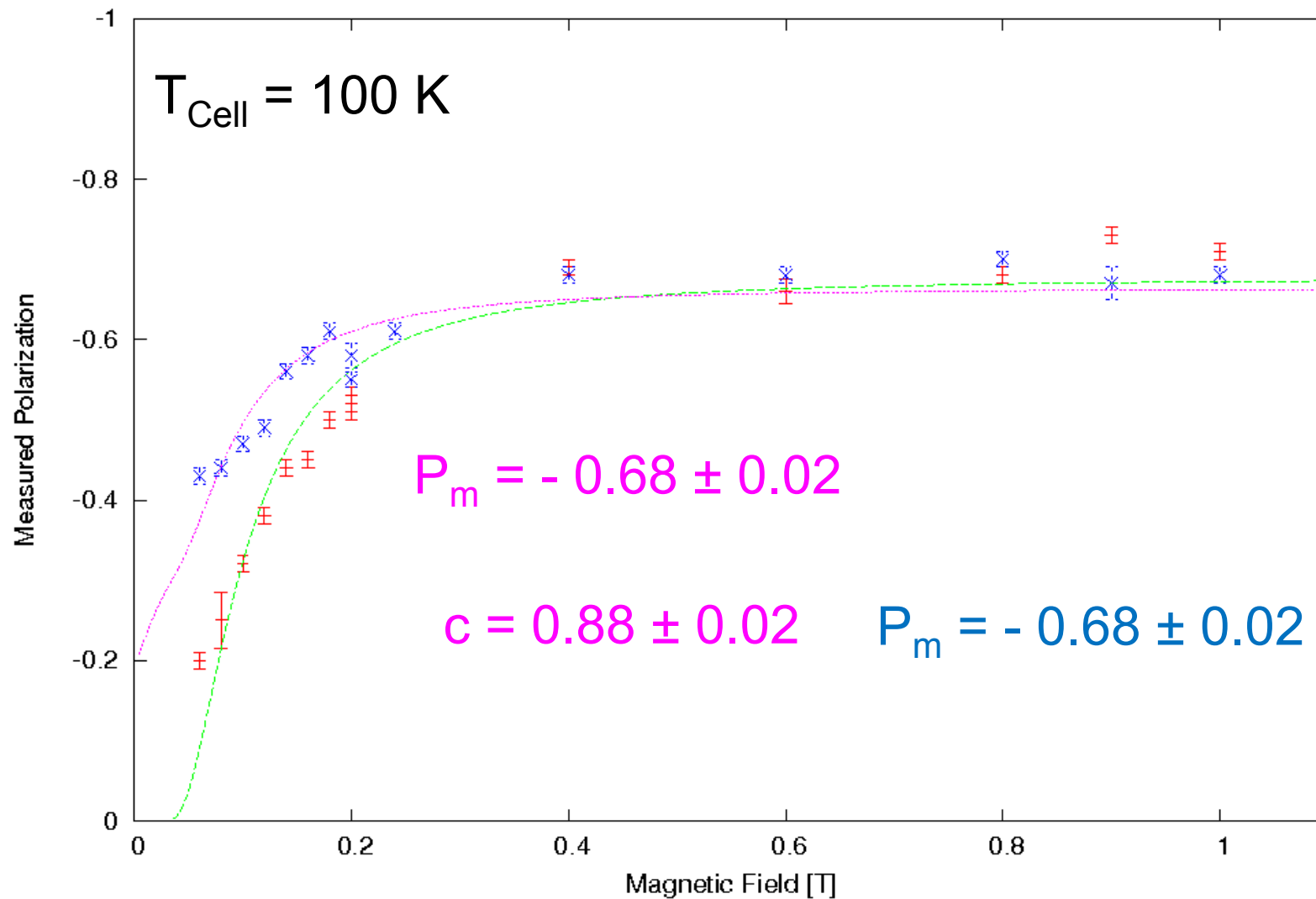
HFS 3: Next attempt



Experimental results

Measurements on Fomblin Oil (Perfluoropolyether PFPE)

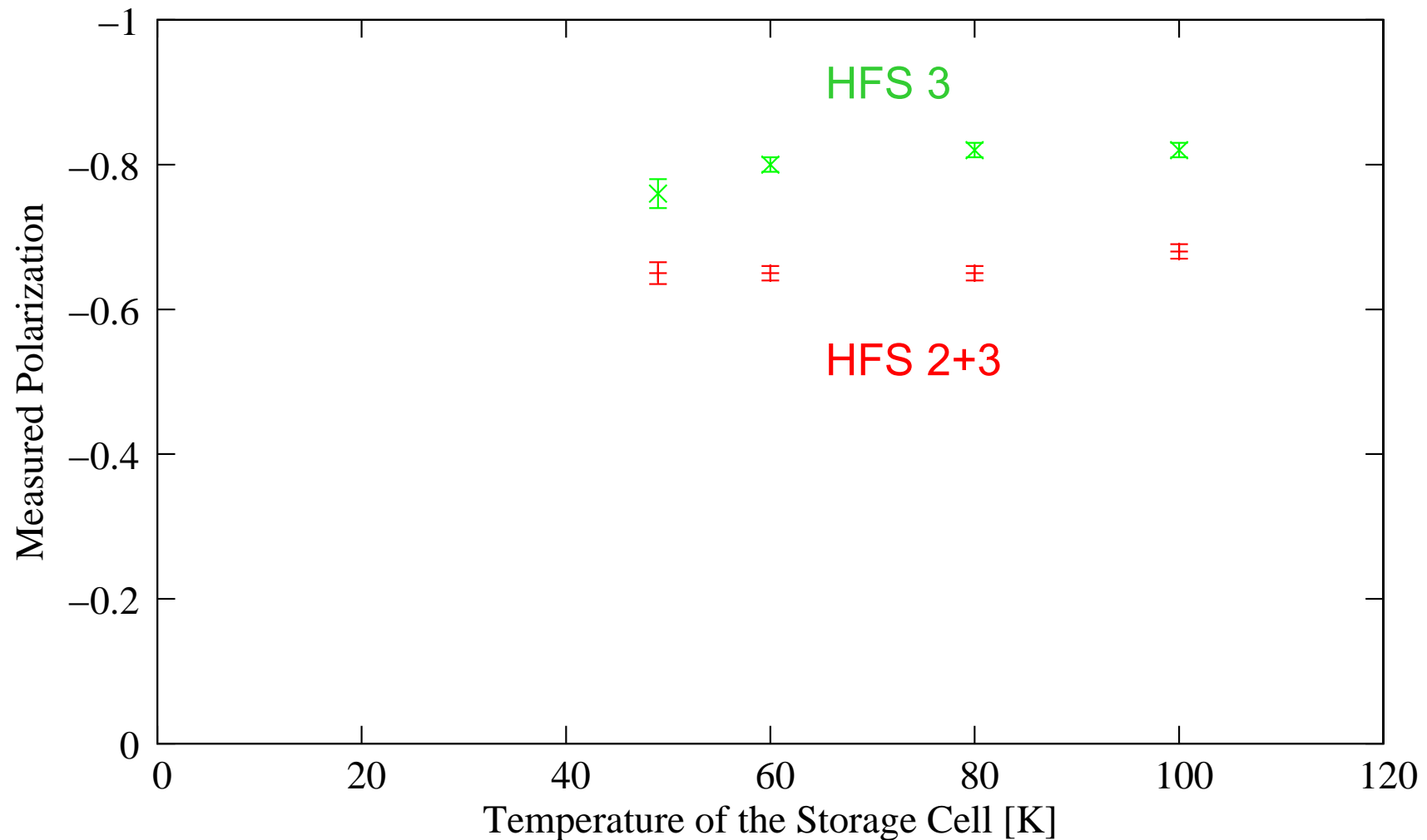
HFS 2+3: Next attempt



Experimental results

Measurements on Fomblin Oil (Perfluoropolyether PFPE)

$B_{\text{cell}} = 0.4 \text{ T}$, H_2^+ only



Conclusion

We can measure:

- the **recombination** of hydrogen/deuterium atoms on different surfaces and for different HFS.
- the **polarization** of **atoms** and **molecules** in a storage cell.
- the **number** of **wall collisions** of the molecules in the cell.
At least, we can see the difference between „hard“ and „soft“ materials (elastic scattering, cos-distribution or \cos^x -distribution).
- the B_c for vector- and tensor-polarized **Deuterium**.

To-do List

- Calculation of B_c for vector- and tensor-polarized Deuterium
- Additional cryo-catcher between ABS and ISTC-chamber
- Measurements on different surfaces:
 - Aluminium
 - Teflon
 - ...
- More measurements on a water surface
(Maybe the surface below has some influence ...)
- Polarized Deuterium Fuel for polarized fusion reactors

Outlook: Polarized Fusion



Advantages:

- 1.) Increased energy gain (ITER: ~ 2 / Megajoule: ~ 4)
or reduced costs for the reactor
- 2.) Focussing of the neutrons on special wall areas
or suppression of the neutrons for a neutron lean reactor
($E \sim B^{7.84}$)

Outlook: Polarized Fusion

Problems to solve:

- 1.) All double-polarized cross sections must be known !
 - > d-d reactions are missing
 - > **Measurements are underway at PNPI**
- 2.) Does the polarization survives in the fusion plasma ?
 - > Laser-induced fusion: Test with pol. ^3He gas is foreseen in 2016
 - > Tokomak: Joined collaboration between Jlab and DIII
- 3.) How to produce and handle polarized deuterium ?
 - > maybe pol. Deuterium molecules can be frozen out, collected and stored for some time

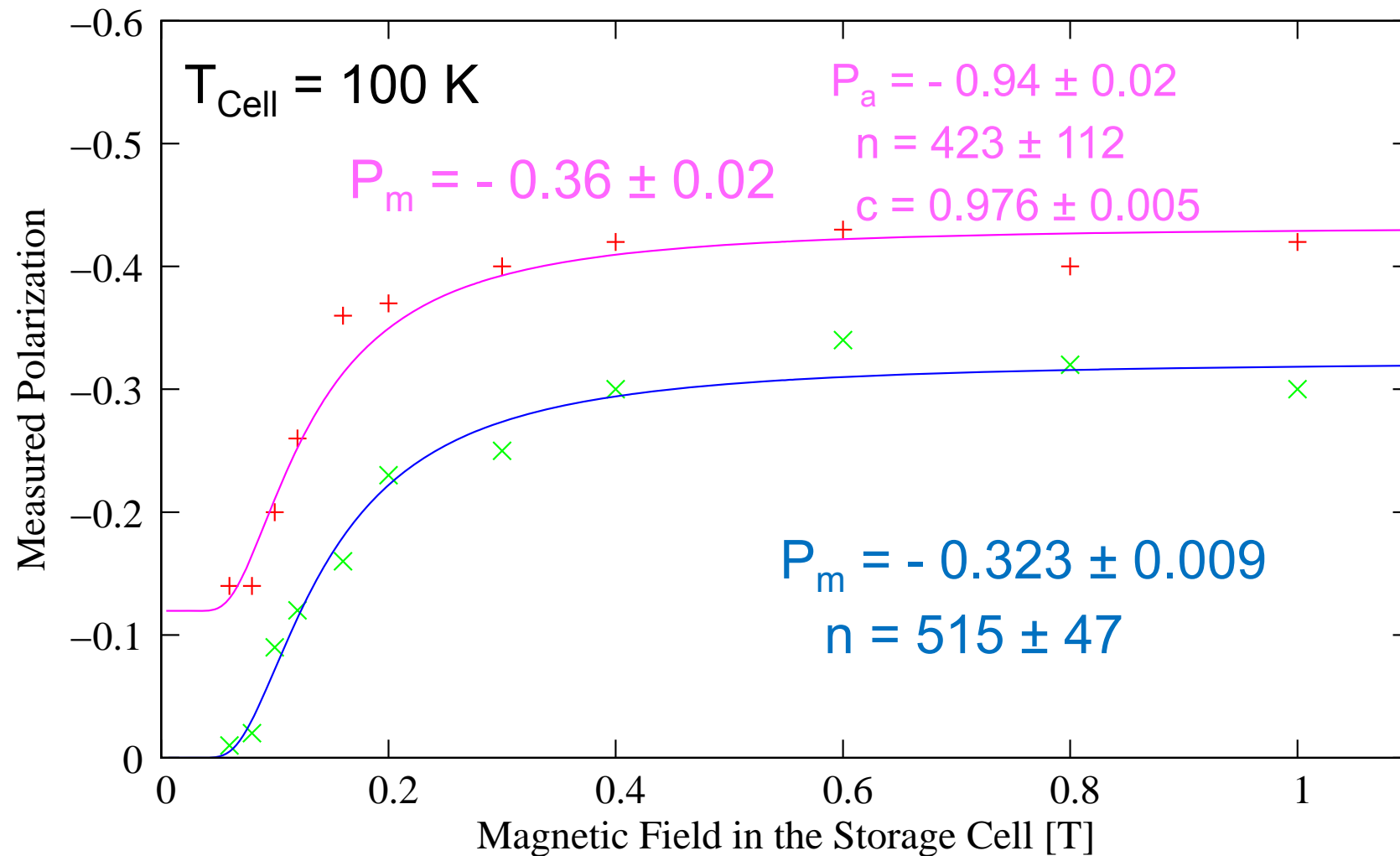
Nicolai Tchernov: First Spokesperson of this ISTC Project



Experimental results

Measurements on Fused Quartz Glass after several days

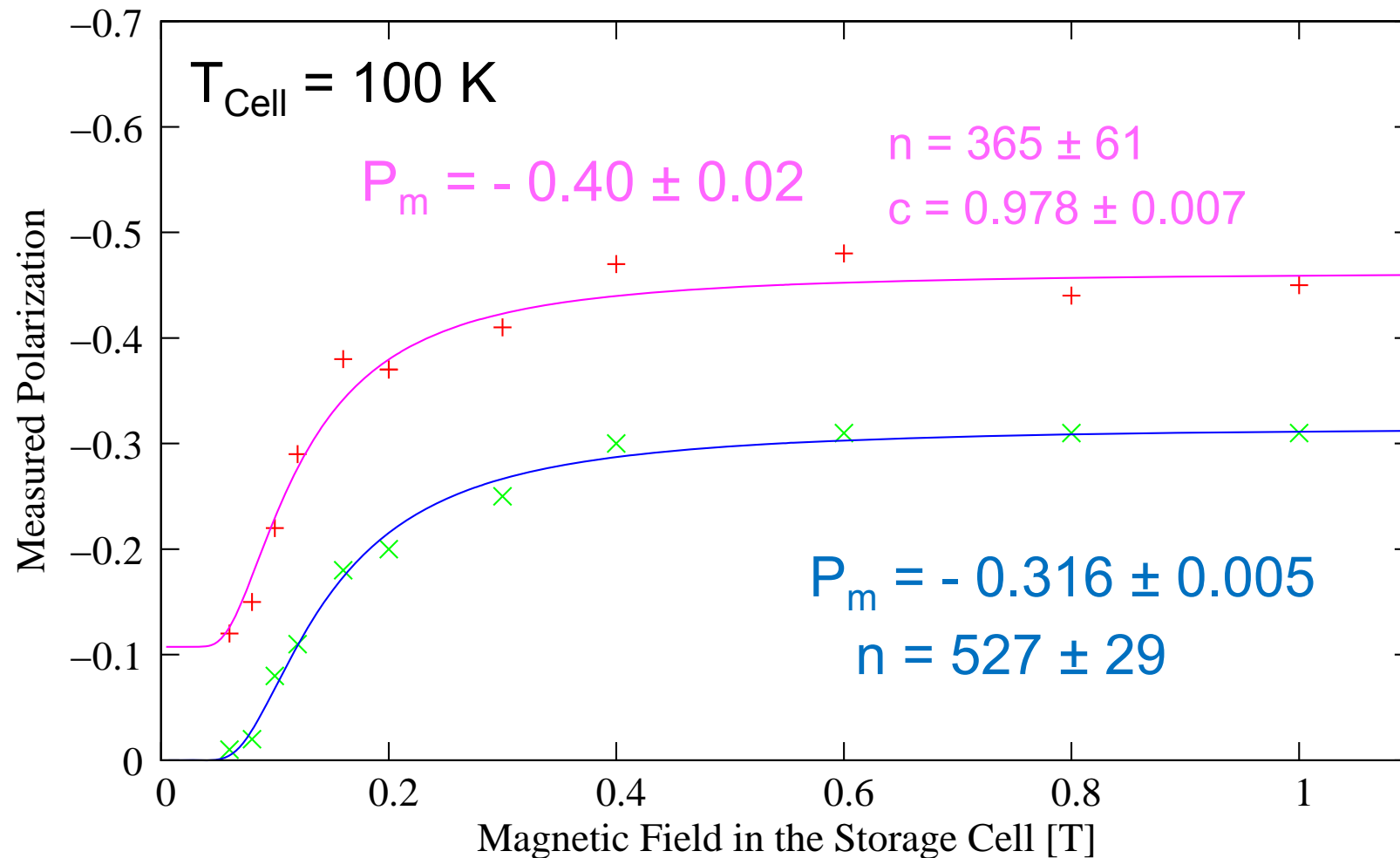
HFS 2+3



Experimental results

Measurements on Fused Quartz Glass after several days

HFS 3



Experimental results

Measurements on Fomblin Oil (Perfluoropolyether PFPE)

